Garvin

NATIONAL BUREAU OF STANDARDS REPORT

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THERMODYNAMIC DATA FOR INDUSTRIAL INCINERATORS

Thermochemistry Section
Physical Chemistry Division
Institute for Materials Research
for
Office of Standard Reference Data

U.S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

NATIONAL BUREAU OF STANDARDS

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Office of Standard Reference Data—Office of Technical Information and Publications—Library—Office of International Relations.

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[1] Headquarters and Laboratories at Gaithersburg, Maryland, unless otherwise noted; mailing address Washington, D.C. 20234.
[2] Part of the Center for Radiation Research.
[3] Located at Boulder, Colorado 80302.

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THERMODYNAMIC DATA FOR INDUSTRIAL INCINERATORS

with

Guides to the Use of the Tables

By
George T. Armstrong
and
Eugene S. Domalski

Final Technical Report
to
American Society of Mechanical Engineers
Research Committee on Industrial Wastes

⟨NBS⟩

U.S. DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

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20.0 Preface

20.1 Introduction

Maintenance of a high-quality clean environment in our current
technological civilization has many facets; however, there is no question
that effective disposal of waste materials is a primary factor in
achieving this desirable goal. The neglect of this perennial, necessary,
housekeeping chore would lead to accumulation of discarded materials in
a way that could not be ignored for reasons of health, safety, efficient
performance of activities, and aesthetic impact. The means of accomplish-
ing the disposal of waste have varied with the state of development of
our civilization and technology and in the most primitive procedures con-
sisted of dumping or dispersal on land, into oceans and lakes, into rivers,
or into the atmosphere.

More sophisticated techniques consist of chemical or physical
processing to modify the form of the wastes and then dumping as before.
Still more sophisticated techniques include chemical or physical pro-
cessing as before, but modified or selected to achieve a goal of partial
or complete re-use of the waste materials.

The initial cost and effort of devising ways to carry out methods
of disposal increased rapidly with their increasing degree of sophisti-
cation. As a result, mostly for economic reasons, the least sophisticated

and most direct means are usually used. Satisfactory and optimum tech-
nological procedures for the more sophisticated means of disposal have
not been developed yet for many forms of waste.

Among the chemical processing techniques of moderate sophistication
incineration ranks as an important and widely used device for converting
wastes to less undesirable forms before dumping or dispersal. Incinera-
tion is applicable to gaseous, liquid, or solid wastes. It reduces the
residual bulk of many solid or liquid wastes, converts most organic
materials into gases which are already part of the natural atmosphere and
can be released directly into it, generates heat which can be used in some
instances, used readily available oxygen or air as its principal chemical
agent, causes chemical processes that are comparatively well understood,
and is readily carried out rapidly on large quantities of materials in
apparatus of comparatively simple design.

Disadvantages of incineration are its generation of some noxious
or toxic gases, smoke, and other atmospheric pollutants unless specially
designed equipment is used, and the low economic value of the products
of combustion. The generation of atmospheric pollutants can be largely
controlled by proper design of the incineration apparatus or by further
processing of the effluent gases before emitting them to the atmosphere.
The ultimate limitation on the usefulness of incineration as a waste
disposal technique (with respect to combustible substances) is probably
going to be the implicit extravagance of its use.

Nevertheless, because of several advantages listed above, incin-
eration as a waste disposal technique is going to be in use for a long
time into the foreseeable future. As indicated above, the proper design

of incinerators is, therefore, environmentally and economically desirable, and, because of legal specifications on emission, may also be required.

The American Society of Mechanical Engineers (ASME) recognized this problem as of growing importance in the light of increasing professional and public awareness of the whole waste-disposal problem and its environmental implications. The ASME Research Committee on Industrial Wastes undertook to provide a guide to the design of industrial incinerators as an ASME publication. In collaboration with a task group of his committee, the National Bureau of Standards through the Office of Standard Reference Data (OSRD) has prepared this compilation of thermodynamic data on potential ingredients and products of combustion of industrial wastes. Some guides to the use of the data for computation of thermodynamic parameters associated with the incineration process are also given. The use of this type of data is essential in the calculation of incinerator design parameters for particular disposal problems.

Incineration will undoubtedly assume a well-defined place in the spectrum of methods available for waste disposal. The field at present is in a state of considerable innovation and flux; but also includes non-combustion chemical treatments, pyrolysis, and atomization. The data and the accompanying guides to their use will probably find application in these areas too because parameters of many of the processes involved can be calculated using the same input thermodynamic data.

20.2 Anticipated Needs for Thermodynamic Data

In the design of industrial waste disposal units, in particular--incinerators, the engineer has two major problems which must be solved

in an internally consistent way in order to obtain satisfactory perform-
ance. (a) The composition of the mix of input materials, which may
consist in general terms of waste, added fuel, and combustion air or
oxygen, must be understood and adjusted in such a way as to allow the
requisite combustion processes to be carried out leading to known pro-
ducts. (b) The heat balance of the process based on energies of com-
bustion (or other reaction) must be known at various stages of the
process, in order to allow proper temperature control to be maintained.
To meet these requirements there is need for a substantial body of thermo-
chemical data for ingredients of waste, either as enthalpy of combustion
or enthalpy of formation at room temperature, and need for some information
on products of combustion at high temperatures such as their enthalpies
of formation, heat capacities and Gibbs energies. These needs resemble
in many ways those which have been met in the past few years for quantities
of thermodynamic data on rather large numbers of substances as for example
in the rocket propulsion program.

Looking at the waste disposal problem from another point of view
one sees that the use of incinerators has two quite different aspects.
In the first instance, mechanical engineers involved in incinerator design
are faced with the problem of obtaining effective combustion and therefore
must know the combustion performance of the materials they put into the
incinerator in an approximate way. Under many existing circumstances a
high degree of precision in the calculations is not required. However a
secondary problem now is known and is likely to be of considerably more
importance in the future. This is the control of noxious substances

emitted by the incinerator which tend to pollute the atmosphere. Because of the human factors involved in the exposure of the public to the emission products and because of federal, state, or municipal control mechanisms which are likely to be specified to limit pollution of the atmosphere, it will be very important ultimately to know the kind of substances that will be present in the products of combustion and to guarantee the upper limits of specified substances. In order to be able to estimate the combustion product concentrations with assurance we anticipate that considerably more accurate knowledge of the enthalpies of formation of the ingredients, and the enthalpies of formation and other thermodynamic properties of a much wider range of products will be required than are needed in the first instance.'

To meet the requirements for thermodynamic data by engineers and designers, a handbook is needed which will provide (a) tables of thermodynamic data applicable to common problems of waste disposal by incineration and (b) guidance in the use of the tables and in obtaining supplementary information. The handbook may appropriately contain a discussion of the application of thermodynamic data to calculation of heat balances, and the effects of the composition of the input materials on the output composition; also, a discussion of the limitations of accuracy of the calculations, and the possible need for more elaborate analysis and more accurate data on input materials if output products must be closely controlled (as for pollution control).

The required tables are enthalpies of formation and Gibbs energies of as large as practical a number of potential input materials at 25°C,

and of potential incineration products at 25°C and elevated temperatures ranging to 2000°C or higher.

An important feature of the presentation of technical data should be a format suitable for engineering use, and rather detailed guidance as to use of the data. In addition, as it is not practicable to include available thermodynamic data on all substances, nor do data exist on all substances that are potentially of interest, it is important to provide two specific supplements to the thermodynamic data: (a) bibliographic references to reliable and extensive collections of data on additional materials, (b) selected lists of methods of estimation of the properties. A discussion of the merits of these referenced collections and methods of estimation will be helpful to the engineer.

20.3 Scope and Preparation of Tables

Following general lines of the discussion presented above, preparation of material for a handbook of thermodynamic data for industrial incinerator design and operation was undertaken.

As an initial step in limiting the coverage of substances to be included, a survey was made by Mr. Wayman L. Calhoun (Union Carbide Corp.) of the ASME Research Committee on Industrial Wastes. The persons queried were primarily members of the Subcommittee on Coordination with Associations and Government. The results of this survey in general indicated the following points:

   (a) A large fraction of the industrial waste to be disposed of
       consists of organic materials which fall generally into
       three categories:

      (1)   pure substances, well defined

      (2)   organic materials of variable composition but

            resolvable into known components

      (3)   poorly defined mixtures

   (b)   A smaller amount consists of inorganic materials. Among

       these, ingredients include essentially all the elements

       in small amounts and some, such as ferrous and non-ferrous

       metals, in relatively large amounts.

On the basis of this survey, the time and effort available, and the desire

to have the tables available in a reasonably short time to enhance their

early usefulness, the final plan for the tables was as follows:

     Enthalpies of formation at 25°C (298.15K) were agreed to be of

primary importance. Tables of thermodynamic functions of temperature

are of less immediate importance as many of these are available in the

extensive JANAF Thermochemical Tables and the computer tapes associated

with them (See source 20, Section 22.0).

     The scope of the substance coverage was established as follows:

   (a) Organic compounds. All organic substances for which experi-

       mental data are available, within the limits of time and

       effort available.

   (b) Organic materials (not well characterized). Limited to

       polymeric substances to which a reasonably good formula

       can be attributed.

   (c) Inorganic compounds. Inorganic oxides, only.

The decision not to list poorly defined materials was made deliberately because of the open-ended nature of the list, the lack of carefully screened sources of data, and the possibility of approximating combustion values from data on related pure substances. The alternative decision was made to include all polymers for which data could be found, as polymeric substances were prominent among the large volume waste products.

For the above three classes of substances enthalpies of formation at 298.15K are provided in tables obtained as described below.

To prepare Table I, "Enthalpies of Formation of Organic Compounds at 298.15 K", advantage was taken of the fact that in the Chemical Thermodynamics Data Center a comprehensive monograph is in preparation for the OSRD. Files of compounds for which enthalpies of combustion have been determined now comprise about 4000 compounds. The data on these have not all been evaluated. The tabulated list, therefore, comprises the 1000 compounds for which work had been completed. The selection of these compounds was made on the basis of (a) important functional groups and, (b) importance of the compound. The selection of appropriate substances was aided by the fact that a recent previous review had been made for NASA in which compounds of primary interest in biology and biochemistry had been selected for early evaluation.

In the selection of values for enthalpies of formation, the data were derived from measured values of enthalpies of combustion, usually performed by bomb calorimetry. The measurements had been made, in some cases, over a period of a hundred years, and hence were of very non-

uniform quality. The data for each substance were evaluated and updated according to uniform criteria, which are described by Domalski (source 4, Section 22.0). They represent the best values that can be derived from existing data.

Because of the prospective repetition of needs to tabulate organic compounds with their enthalpies of formation and other data, a permanent, machine-readable file was organized during the course of this work. The final listing of compounds which forms Table I was prepared from this file.

To prepare Table II, "Enthalpies of Formation of Organic Polymers at 298.15 K", the Chemical Thermodynamics Data Center file of enthalpies of combustion of organic compounds was combed for relevant substances. Recent reviews of enthalpies of formation of organic polymers were also searched. All polymers were included for which reliable enthalpies of formation could be determined from their enthalpies of combustion. The final table comprises 39 polymers.

The values listed in Table II were arrived at in the same way as those in Table I; hence, they represent the best values available on the basis of existing experimental data.

To prepare Table III, "Enthalpies of Formation of Inorganic Oxides at 298.15 K", the recent set of NBS compilations of critically evaluated data on the thermodynamic properties of inorganic substances was the principal source. These tables (NBS Technical Note 270, D. D. Wagman, et al., 1965-1971 and continuing) are the most recent comprehensive critical evaluation on inorganic compounds, and have the title "Selected

Values of Chemical Thermodynamic Properties". Oxides for which enthalpies of formation were known to have been determined, but not yet found in completed sections of TN 270 were obtained principally from the JANAF tables. References to the sources of data are given appended to Table III.

Each of the sources listed above is a tabulation of values by competent reviewers who have devoted years of systematic study to the selection and evaluation of chemical thermodynamic data. The tabulations quoted in each case are authoritative and may be said to represent the best values available on the basis of existing experimental data. Only one or two estimated values have been included.

The prepared descriptive material consists of:

(a) general background of thermodynamic definitions and formulas necessary to an understanding of the discussion; (b) detailed discussion of the calculation of thermodynamic quantities at 298.15 K, using the material from the tables; (c) a brief general discussion of calculations involving elevated temperatures; (d) supplementary sources of thermodynamic data, and methods of estimation, and (e) an appendix giving auxiliary constants, symbols, and units of measurement.

20.4 Status of Thermodynamic Data and Auxiliary Aids: Recommendations for Further Action

Listed below are the stronger impressions obtained concerning needs for information as compared with its availability and completeness. A few recommendations are made for action to alleviate some deficiencies or fill certain needs.

1. A large category of ingredients for incinerator processes was found to be "poorly characterized materials": materials which by dint of some effort could be resolved into well defined substances, and materials for which this might not even be possible. These materials are not included in the tables for the handbook. However, the practical incinerator process manager is going to need information to allow him to make ad-hoc decisions. This information can take the form of (a) tables of classes of ingredients of typical poorly characterized materials, together with appropriate elemental composition and enthalpies of combustion or a pseudo-enthalpies of formation; (b) tables of enthalpies of combustion or pseudo-enthalpies of formation of well known classes of materials for which only average values can be cited. Such materials as coal, hard-woods, soft-woods, petroleum oils, fall in this category. The accuracy of the enthalpy values may not be high, but the elemental composition and a pseudo-enthalpy of formation would allow such materials to be fed into computer programs for calculating high temperature equilibria as well as any well-defined substance. Only the products of combustion enter the final equilibria, and their proportions will be fixed by the proportions of the elements and parameters independent of the nature of the combustible material.

2. In reviewing the reactions for possible combustion reactions involving water and various volatile acids, it became apparent that conditions of operation of an incinerator (for example: using scrubbing water on effluent gases) can be readily envisioned which will require vapor-liquid equilibria of a few volatile acid-water solutions. The

relevant data include such parameters as partial pressures of HCl and H_2O as functions of temperature and mole ratios for solutions of HCl in water. Other acid gases such as HF, SO_2, SO_3, P_4O_{10}, N_2O_5 also enter such equilibria. Satisfactory data for these equilibria probably exist, but could not be organized within the scope of this project.

The number of organic substances for which enthalpies of combustion are known is much larger than those tabulated. The critical review of the data is proceeding rapidly, and a much longer list will be available in perhaps two years. The list given as Table I could then be augmented.

A serious deficiency exists in the availability of experimental enthalpies of combustion (and formation) of organic polymers. This is made quite obvious by the availability of reliable combustion data for only 39 out of the multitude of polymers in large scale industrial use. More experimental values are needed on these large-volume chemicals, to provide additional data for an augmented Table II. There are also other important uses for such data.

20.5 Collaborative Arrangements

As the administrators of the National Standard Reference Data System (NSRDS), the Office of Standard Reference Data (OSRD) at NBS (Dr. D. R. Lide, Director) agreed to provide the handbook materials to ASME for its Research Committee on Industrial Wastes (E. S. Monroe, Chairman). The working organization within NBS which was assigned by OSRD to carry out the project was the Thermochemistry Section of the Physical Chemistry Division, Institute for Materials Research. Dr. George T. Armstrong and Dr. Eugene S. Domalski carried out the work,

using the resources of the Chemical Thermodynamics Data Center (Mr. D. D.
Wagman, Manager), which is organizationally located in the Thermochemistry
Section.

The organization of the work was planned by Mr. E. S. Monroe
(E. I. du Pont de Nemours and Company, Inc.), Mr. R. A. Conway (Union
Carbide Corp.), Mr. W. L. Calhoun (Union Carbide Corp.) and Dr. S. R.
Beitler (Director of Research, A.S.M.E.) all representing the A.S.M.E.,
and by Dr. H. J. White, (OSRD), Dr. George T. Armstrong, Chief, Thermo-
chemistry Section, Dr. C. W. Beckett, Physical Chemistry Division Office,
and Dr. David Garvin, Coordinator of Data Programs for the Physical
Chemistry Division Office. During the early part of 1971, after the
project was started, Mr. F. H. Small (Union Carbide Corp.) replaced
Mr. Conway.

During the course of the work, continuing guidance was received
from the ASME Research Committee on Industrial Wastes. Assistance from
the staff of the Chemical Thermodynamics Data Center, in particular
Mrs. J. J. Grimes and Miss B. Beckwith is acknowledged, in setting up
a mechanism for information storage and retrieval of enthalpies of
formation of organic compounds, and from Mr. J. I. Minor of the Thermo-
chemistry Section in processing the data files.

21.0 Discussion and Aids for the Use of the Tables

21.1 Processes Occurring in Incinerator Combustion

Thermochemical and thermodynamic data have well de-
fined applications in the analysis of incinerator processes
and in the design of incinerators. The energy released
during the combustion process appears as heat. This heat
causes the gases formed in the reaction to be hot, and the
non-volatile materials to form hot ash, cinders, or molten
refractory materials. It may be carried away in hot effluent
gases or by conduction through the walls. The heat must be
under control in that the incinerator must be designed to
withstand it, and possibly, by heat exchangers, to make use
of it in an auxiliary operation. This heat may be used to
volatilize non-combustible substances in the ingredients,
such as water, which needs only to be volatilized in order
to make it an acceptable effluent into the atmosphere. Under
any circumstances the heat will be carried away from the
reaction zone; and the mechanism by which this is to be done
is an important part of the incinerator design. The reaction
processes may require supplementary heat or possibly damping
in order to make the combustion complete or to provide gaseous
or solid products as appropriate at the end of the process.
Information required for the calculation of these processes
are the nature of the ingredients and products, and the
values of their enthalpies of formation, heat capacities
or enthalpies of the products as functions of temperature.

The heat of the reaction may cause some of the products formed to be partially or completely dissociated. The temperature to which the effluent gases and the residues are heated, and the nature of the products found in them are determined to a large extent by the dissociation equilibria and other equilibria that can occur as a result of interactions between the products of combustion. The proportions of materials present in the products are strongly dependent upon the equilibrium constants of the various possible reactions. The important thermodynamic data here are the Gibbs (free) energies of formation and the equilibrium constants of formation of the products of reaction at the possible temperatures. The occurrence of spontaneous reactions in a constant pressure system is governed by a decrease in Gibbs energy; and the equilibrium proportions of substances present are determined (as the equilibrium constant) from sums of the Gibbs energies of formation from the elements. Available data may be the Gibbs energy or it may be enthalpy and entropy data from which the Gibbs energy may be calculated. The equilibria are strongly temperature dependent; hence there are strong connections among the enthalpy of reaction, the heat capacities of the substances, heat retention in the incinerator, and the proportions of products that will be present following the reaction.

A third area of importance of the thermodynamic data
is in the possible interaction of ingredients or products
of combustion with the materials of construction of the in-
cinerator. Here much more flexibility occurs. The materials
to be burned may be relatively fixed before incinerator de-
sign is attempted, or on the other hand the variety of ma-
terials may be very great. The selection of materials of
construction may depend upon knowledge of volatility or re-
fractoriness of substances possibly to be formed by inter-
action of the hot incinerator gases with the walls.

Thermodynamic data applicable to the solution of some
of these problems are discussed in the following parts of
Section 21. This presentation and some general principles of
their use is not an attempt to recommend methods for cal-
culation of specific incinerator design parameters, but rather
to provide a ready reference to the meaning and typical ap-
plications of thermodynamic data of special value in such
applications.

21.2 Definitions of Thermodynamic Terms

21.2.1 Temperature. Temperature is a measure of the hotness
of a system. Note: A system may be a given quantity of a
single substance, or it may be a complex mixture or aggregate
of material.

When analyzed in terms of the motions of the atoms or molecules
constituting a material, the temperature is a measure of the

average kinetic energies of their random movement. Sub-
stances in a system and all parts of a system tend to ap-
proach the same temperature, and will attain the same tem-
perature if disturbing processes are absent.

The temperature occurs as a parameter of importance in
all heat transfer processes, in chemical reaction processes,
and in the properties of materials and chemical substances.

All thermodynamic formulas and laws involving tem-
perature with a basis in theory require temperature to be
expressed in terms of the thermodynamic or absolute tempera-
ture scale. The internationally agreed version of the ther-
modynamic temperature scale is the International Practical
Temperature Scale. The kelvin (symbol K) is the unit of tem-
perature and the size of the kelvin is determined by defining
the temperature of the triple point of water as 273.16 K.
The freezing point of water (melting point under 1 atm pressure
of air) is defined as 0.01 K below the triple point, hence
the normal ice point is 273.15 K.

The ice point temperature is 0°C on the frequently
used Celsius (centigrade) temperature scale. The size of
the temperature units is the same on the Celsius and the
thermodynamic scales. The relationship between the scales
is expressed by the equation

$$t = T - 273.15$$

where t is the temperature (°C) on the Celsius scale, and T is
the temperature (K) on the thermodynamic scale.

21.2.2 Energy of a System

Every physical system has associated with it a certain amount of energy which is variously described in terms of several state functions--internal energy, enthalpy, Gibbs energy, or Helmholtz energy--depending upon the use to which the information is to be put.

The energy of a system is an extensive parameter; that is, the amount of energy is proportional to the mass (kilograms) or the amount (moles) of each substance present.

> Note: The unit of energy is the joule (symbol J), though values are commonly given also in calories (symbol cal) and, in engineering practice are sometimes given in British thermal units (symbol Btu). The amount of substance referred to in an equation is in terms of moles (symbol mol). In this handbook, unless otherwise specified, a tabulated enthalpy, or other thermodynamic quantity attributed to a particular substance is for a mole of that substance as described by its formula. The mass corresponding to a mole is found by taking the molecular weight is n grams. The engineering unit pound mole (symbol lb-mol) is not used in this handbook. See Appendix section 25 for definitions of the units of measure and for relationships between the units.

21.2.3 State Function

State functions are any of several extensive thermodynamic functions, relating to the energy of a system, of which the values are uniquely defined for a given system when its state is defined. These include internal energy, enthalpy, Gibbs energy, Helmholz energy, entropy, and some functions derived from them. The state of a system is defined when

it is at equilibrium in a given physical state at a given temperature, and under a given set of external stresses, such as a given pressure. The important feature of a state function is that the value does not depend upon the path by which the specified state of the system is reached. Put in another way, the difference in value of a state function in two states of a system is independent of the path by which the system is changed from one state to the other.

It should be noted that all the state functions defined below are not required for direct use in incineration design. However, they need to be defined here, because of their uses in tabulation of thermal data (see Sec.21.3) in some of the auxiliary reference sources to be cited later.

21.2.4 Internal Energy

A system is said to have internal energy (symbol U) which changes as heat is added or removed, and work is done on or by the system. While the absolute value of the internal energy of a system is arbitrary, and unimportant for the purposes of thermodynamics, changes in internal energy can be measured. The equivalence of heat and work in their influence on the internal energy of a system is expressed by the equation

$$\Delta U = q + w$$

In the above equation, ΔU represents a change in internal energy. An increase ΔU in the internal energy of a system

may be caused by supplying an amount of heat, q, to the
system and doing an amount of work, w, on the system. The
two quantities, w and q, are not state functions, but depend
on the path followed. They have the same energy units,
may be applied simultaneously or sequentially, and may have
any values relative to one another. The direction of heat
and work transfer as denoted by their signs must be chosen
in a consistent manner. There is no universally accepted
convention as to the signs of heat and work energy supplied
to a system, so care should be taken to note the convention
used in any particular presentation.

The internal energy is a function of temperature, pres-
sure, and other parameters, which has a characteristic value
for a fixed amount of a particular substance in a defined
state. Another common symbol for internal energy is E.

In a reaction carried out at constant volume the heat
effect of the process measures a change ΔU (or ΔE) in the sub-
stances. If heat is produced by the reaction (exothermic
reaction) the change ΔU is negative. An engineer examining
combustion measurements made in a bomb calorimeter may find
the data expressed as ΔU or ΔE as this is a constant volume
process.

21.2.5 Enthalpy

The enthalpy, sometimes called heat content, (symbol H),
of a system is a measure of its energy which differs from the

internal energy by the amount of work done by the system against the pressure of the surrounding medium. The enthalpy is defined by the following relationship

$$H = U + pV$$

in which U is the internal energy, p is the pressure of the surrounding medium, and V is the volume of the system. The enthalpy and the internal energy of a system are the same when the pV term is zero. This occurs only when (1) the system is a condensed phase and the external pressure is zero, or (2) when the system is an ideal gas at the absolute zero of temperature.

In a constant pressure process, (i.e. a process in which initial and final pressure are the same) the change in enthalpy is given by the following equation

$$\Delta H = \Delta U + p\Delta V$$

The change in enthalpy associated with a process is equal to the change in internal energy only when (1) the pV terms are all zero as above, or (2) when the volume of the products is the same as the volume of the reactants.

As in the case of internal energy, the absolute value of the enthalpy is arbitrary and only changes in enthalpy can be measured.

For processes occurring at constant pressure, such as combustion at normal atmospheric pressure, if the products are cooled to the starting temperature, the heat effect observed

is the enthalpy change ΔH. For an exothermic reaction ΔH
is negative. See Section 21.5 for illustrations of cal-
culations of ΔU and ΔH.

When two molecular species in a system react to form
another molecular species, such as

$$H\text{-}H(g) + Cl\text{-}Cl(g) \rightarrow 2H\text{-}Cl(g)$$

and the reaction is exothermic (ΔH is negative) we can
say that the molecular arrangement of the products is more
stable, or gives stronger bonds than those of the reactants.
This excess energy released by forming the stronger bonds
becomes available and may be released as heat. A decrease
in internal energy, or enthalpy is a driving force which
tends to cause a process to occur spontaneously (in order
to arrive at a more stable state), but though it is a dominant
effect, it is not sufficient in itself.

21.2.6 Entropy

The entropy (symbol S) is a measure of the disorder
or randomness in a system. Another way of putting it is
that the entropy of a system is directly related to the
number of states of existence available to it. If the
number of states of existence for a collection of atoms is
greater in one molecular configuration than in another con-
figuration the entropy will also be greater. The difference
in the entropy of liquid water and gaseous water may be used
as an example. When water is condensed to liquid its

molecules have much less freedom of movement than when the water is a gas. The gas molecules have many more configurations available to them, and so at a given temperature the entropy of a given amount of water vapor is much greater than that of the same amount of water liquid.

Heating a body reversibly increases its entropy by an amount equal to the quantity of heat divided by the absolute temperature. Thus an infinitesimal amount of heat, δq, supplied reversibly increases the entropy of a body by $d\delta$ where

$$d\delta = \frac{\delta q}{T}$$

For a given substance the kinetic, rotational, and vibrational movement of the molecules increases with temperature. The amount of disorder therefore increases with temperature and the entropy of a substance is greater at a high temperature than at a low temperature.

The tendency for entropy to increase is a driving force which causes processes to occur spontaneously, but is not sufficient in itself. It is usually not sufficient to overcome an opposing energy change and where it is sufficient we will have a spontaneous endothermic process. The entropy in any closed system tends to increase with time, with an ultimate maximum when equilibrium has been reached.

When reactions are carried out rapidly and under nonequilibrium conditions, hence irreversibly, as is the common practice in rapid combustion, the increase in entropy of the

whole system is always greater than that calculated for
the reversible reaction.

21.2.7 Free Energy

See Gibbs Energy; see also Helmholtz Energy.

21.2.8 Free Energy Function

See Planck Function; see also Massieu Function

21.2.9 Helmholtz energy

The Helmholtz energy (symbol A) is a measure of the
maximum work that can be done by a system. It is defined by
the equation

$$A = U - TS$$

The change in Helmholtz energy that occurs in a process at
constant temperature is given by the equation

$$\Delta A = \Delta U - T\Delta S$$

In an isothermal process, the maximum amount of work that can
be done by a system is $-\Delta A$, the decrease in Helmholtz energy.

The Helmholtz energy is a valid measure of the tendency
for a process to occur spontaneously. For a process occurring
at constant temperature and constant volume, the necessary
condition for the process to occur spontaneously is a de-
crease in the Helmholtz energy.

$$\Delta A < 0$$

For an isothermal process occurring at constant volume the
necessary condition for equilibrium is that

$$dA = 0$$

The Helmholtz energy may be found referred to as <u>Helmholtz free energy</u> or <u>Helmholtz function</u>. It should not be confused with the Gibbs energy discussed below.

21.2.10 Massieu Function

The Massieu function (symbol J) is the negative of Helmholtz energy divided by temperature ($J = -A/T$). The Massieu function does not contain any new information not found in the Helmholtz energy; but it is a useful form for calculation of equilibrium processes at constant volume. The Massieu function is found less commonly tabulated than its Gibbs energy analog, the Planck function.

21.2.11 Gibbs Energy

The Gibbs energy (symbol G) is a measure of the maximum work that can be done by a system. It is defined by the equations:

$$G = U + pV - TS = H - TS$$

The change in Gibbs energy that occurs in an isothermal process at constant pressure is:

$$\Delta G = \Delta U + p\Delta V - T\Delta S = \Delta H - T\Delta S$$

For the isothermal process, the maximum work other than expansion work that can be performed by a system is $-\Delta G$, the decrease in Gibbs energy.

The Gibbs energy is also a valid measure of the tendency for a reaction to occur spontaneously. For an isothermal

process subject to a constant pressure, the necessary con-
dition for the process to occur spontaneously is a decrease
in the Gibbs energy

$$\Delta G < 0$$

For an isothermal process subject to a constant pressure,
the necessary condition for equilibrium is that

$$dG = 0$$

An important consequence of this condition is that the
Gibbs energy provides one criterion for the maximum temperature
reached in a combustion zone. At the temperature of the
combustion zone the proportions of substances present will
be governed by the fact that this isothermal Gibbs energy
change will be zero for each possible reaction. That is
each reaction will establish an equilibrium at that temperature.
See Section 21.7 for discussion and an example.

The Gibbs energy is frequently found referred to as
merely _free energy_, and any references to free energy without
qualifying adjectives should be taken to mean Gibbs energy.
It is also called _Gibbs free energy_ or _Gibbs function_ by some
users.

21.2.12 Planck Function

The Planck function (symbol Y) is the negative of Gibbs
energy divided by temperature (-G/T). The Planck function
does not contain any new information not found in the Gibbs
energy; but it is a very useful form for calculation of

equilibrium processes at constant pressure. (See Section 23.3.2). The Planck function is more commonly referred to as free energy function. The terms fef or Gibbs energy function are also sometimes found referring to this function.

21.2.13 Heat Capacity

The heat capacity is the ratio of the energy supplied to the temperature change of a body. It may be an average heat capacity over a temperature range or the limiting ratio over an infinitesimal temperature change. If the system is maintained at constant pressure, the heat capacity, Cp, is the rate of change of enthalpy with temperature.

$$\left(\frac{\delta q}{\delta T}\right)_p = Cp = \left(\frac{\delta H}{\delta T}\right)_p$$

If the system is maintained at constant volume, the heat capacity, Cv, is the rate of change of internal energy with temperature

$$\left(\frac{\delta q}{\delta T}\right)_v = Cv = \left(\frac{\delta U}{\delta T}\right)_v$$

The heat capacity allows one to calculate temperature changes to be expected from liberation of specified amounts of heat, or the amount of heat needed to create a given temperature change.

21.2.14 Enthalpy of Reaction (Heat of Reaction)

For a reaction that goes to completion, the enthalpy of reaction at constant temperature is the negative of the observed calorimetric heat when carried out at constant

pressure and with the products brought to the same tem-
perature as the reactants. It could be logically con-
sidered to be the sum of the enthalpies of the products
of reaction minus the sum of the enthalpies of the re-
actants.

This concept, however, leads to a practical diffi-
culty. The enthalpies of individual substances are based
on arbitrary scales and cannot be added or subtracted
without adjustment. This adjustment is made by relating
the enthalpy scales of various substances through their
enthalpies of formation (heats of formation) (See Section
21.2.15 . On this basis the enthalpy of reaction is the
sum of the enthalpies of formation of the products minus the
sum of the enthalpies of formation of the reactants. If the
sum of the enthalpies of formation at the temperature of
interest is less after the reaction than before, then the
enthalpy of the system has been reduced and the excess
enthalpy will have appeared as heat.

For reaction (1)

$$A + B \rightarrow C + D$$
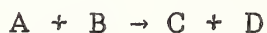
$$\Delta Hr = \Delta Hf[C] + \Delta Hf[D] - \Delta Hf[A] - \Delta Hf[B] \qquad (1)$$

In the example, ΔHr is the enthalpy of reaction, and the
other enthalpy terms are the enthalpies of formation of the
substances contained in the brackets. A negative enthalpy
of reaction means that the reaction is exothermic while a

positive enthalpy of reaction means that the reaction is endothermic.

21.2.15 Enthalpy of Formation (Heat of Formation)

For the special case in which a single product is formed and the reactants are the elements in a standard reference state defined for each element, the enthalpy of reaction is called the enthalpy of formation, and has the symbol ΔHf.

For reaction (2)

$$H_2(g) + \tfrac{1}{2}O_2(g) = H_2O(liq) \qquad\qquad (2)$$
$$\Delta Hr = \Delta Hf[H_2O(liq)]$$
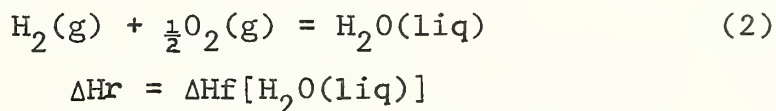
ΔHf, which has a characteristic set of values for any substance is a very important thermodynamic function. The enthalpy change occurring in any reaction can be calculated if the enthalpies of formation are known for all the substances participating as reactants or products. By convention the enthalpies of formation of the elements in their standard reference states are zero, at any temperature (see Section 21.2.16 . An element not in its standard reference will, in general, have a non-zero enthalpy of formation. The standard reference state for hydrogen is the gas composed of molecules, $H_2(g)$. On the other hand the gas consisting of hydrogen atoms $H(g)$ is not the standard reference state for hydrogen. Thus $\Delta Hf°[H(g)]$ at 298K = 52.04 kcal mol^{-1} while $\Delta Hf°[H_2(g)] = 0$, at all temperatures.

21.2.16   Thermodynamic Standard States and Standard Reference
          States

The molal values of the internal energy, enthalpy,
Gibbs energy, Helmholtz energy, entropy, heat capacity and
enthalpy of formation are functions of the temperature. For
simplicity and convenience the values that these thermody-
namic properties have for particular substances are usually
tabulated for the substances in their standard states (indi-
cated by a superscript zero on the thermodynamic symbol as
in ΔHf°, Cp°, etc. The standard states are defined as follows:
For a pure solid or liquid the standard state is the substance
in the condensed phase under a pressure of one atmosphere.
For a gas the standard state is the ideal gas at a pressure
of one atmosphere. For the functions ΔHf, ΔGf, and log Kf
the values tabulated usually represent the quantities appro-
priate for the reaction by which the substance is formed in
its standard state from the elements in their standard
reference states. The conventional notations in this case are
ΔHf°, ΔGf°, log Kf°. For this purpose, in the usual case,
the standard reference states of the elements are taken to be
the molecular form and phase that are stable at one atm pres-
sure at 25°C (298.15 K). A few of the elements, oxygen,
nitrogen, hydrogen, fluorine, and chlorine, are diatomic gases
under these conditions. The inert gases (He, Ne, etc.) are
monatomic gases. Bromine and mercury are liquids. For the
solid elements the stable crystal phase at 298.15 K is the

standard reference state. The single exception to this is phosphorus, for which white crystal phosphorus is used because the more stable forms have not been well characterized thermochemically. In the use of any tables other than those in this handbook, care should be taken to understand the standard states used for the elements, as there is some non-uniformity in this, particularly at temperatures different from 25°C.

21.3 Tabulated Thermal Functions

Tabulated values for the thermodynamic functions are given in terms of carefully defined observables that can be evaluated by experimental means or derived easily by unambiguous calculation from experimental and theoretical relationships. The functions discussed up to this point such as internal energy, enthalpy, Gibbs energy, Helmholtz energy, and entropy suffer from vagueness, particularly with respect to the energy base to which they are referred, but also in other ways. The tabulated thermal functions found in this handbook and in the references given in Section 22.0 are designed to avoid such vagueness. The same criteria are not used in every tabulation, however. It is important to note certain descriptive features of the terminology in order to distinguish the basis of the values in a particular set of tables. When differences in the function descriptions are

noted, in some cases they are unimportant for many calcu-
lations, but in other cases are very important. The principal
distinctions that may be observed are given below, with
some notes as to their importance in particular applications.

Because changes to achieve international uniformity
have been made just recently, many tables which had been
published present the thermal functions in terms of an older
and still widely used system of notation. The principal
identities are

$$E = U \; ; \; F = G$$

The symbols E and F represent the Lewis and Randall (Reference
14, Section 22.0) notations. U and G represent the IUPAC
or IUPAP notation. Practically all earlier tables for Gibbs
energy and various derivative functions of it published in
the United States use the symbol F and the term free energy
for Gibbs energy. The same tables usually use E for internal
energy.

21.3.1 Non-Standard-State vs. Standard-State Functions

The superscript zero is placed by a function to indicate
that the substance is in the standard state. The presence
of a superscript zero by a standard-state function and its
absence by a non-standard-state function should be deliberate
distinctions, though this is not always made clear in the
presentation of a table. U as compared to U°, H vs H°, G vs
G°, Cp vs Cp° differ by amounts that are usually small for

liquids and solids near 1 atm pressure, because of their low compressibility. They become important at high pressures and in the region of the critical temperature. For gases the differences should not be ignored. In this case, the distinction is between the real gas and the ideal gas. For detailed energy balances the real gas state is preferable. Unfortunately real gas functions are unavailable for large numbers of substances. However, the steam tables (Section 22.0, References 2, 7, 8, 13), and the NBS Tables (Section 22.0, Reference 5) apply to real gases.

21.3.2 Different Temperatures for the Energy Base

Internal energy, enthalpy, Gibbs energy, Helmholtz energy, entropy, and certain derived functions are cumulative functions of temperature; and the numerical value given to them, therefore, represents an increment as the temperature of the substance is changed from some reference temperature. The commonly used reference temperatures are 0 K and 298.15 K (The subscript 298 is often used in referring to 298.15 K).

(a) The quantity tabulated for internal energy may be

$$U^\circ - U^\circ_0 \text{ or } U^\circ - U^\circ_{298}$$

depending on the base of temperature used. These two quantities differ by a constant term:

$$(U^\circ - U^\circ_0) - (U^\circ - U^\circ_{298}) = (U^\circ_{298} - U^\circ_0)$$

The quantity $(U^\circ_{298} - U^\circ_0)$ may be found tabulated occasionally.

(b)   The quantity tabulated for the enthalpy may be

$$H° - H_0° \text{ or } H° - H_{298}°$$

depending on the base of the temperature used.   These two quantities differ by a constant term:

$$(H° - H_0°) - (H° - H_{298}°) = H_{298}° - H_0°$$

The quantity $(H_{298}° - H_0°)$ may be found in many tables.

(c)   The quantity tabulated for entropy is usually

$$S° \text{ or } S° - S_{298}°$$

The quantity $S°$, rather than $S° - S_0°$ is usually tabulated on the assumption that $S_0°$ can be exactly determined.   It is usually zero, but may be a constant non-zero quantity.   The difference between the above terms is $S_{298}°$; and this is found in many tables.

(d)   The quantity tabulated for Gibbs energy is usually

$$G° - H_0° \text{ or } G° - H_{298}°$$

The base $H_0°$ instead of $G_0°$ is chosen because the relationship $G_T° = H_T° - TS_T°$ gives us $G_0° = H_0°$ when $T = 0$.
The terms differ by the constant term $(H_{298}° - H_0°)$, which as mentioned above, may be found in some tables.

(e)   The quantities usually tabulated for the Planck function $(-G/T)$ are

$$-(G° - H_0°)/T \text{ or } -(G° - H_{298}°)/T$$

These quantities differ by the amount

$$-(H_{298}° - H_0°)/T$$

which is not a constant, since T is in the denominator.

Despite its anomalous character the function $-(G° - H°_{298})/T$ is very useful, because it allows calculations to be made involving processes for which $\Delta H°_{298}$ is known. These include enthalpies of reaction, enthalpies of phase transition, and so on. Such calculations are quite practical with this function even if the quantity $H°_{298} - H°_0$ may never have been measured, as would be necessary to obtain $-(G° - H°_0)/T$. The negative function is used for the Planck function because most table entries then become positive.

(f) The quantities tabulated for enthalpy of formation (ΔH_f) are

$$\Delta Hf°(\text{at } 0 \text{ K}) \text{ and } \Delta Hf°(\text{at } 298.15 \text{ K})$$

These quantities differ by the amount

$$\Delta Hf°(\text{at } 298.15 \text{ K}) - \Delta Hf°(\text{at } 0 \text{ K}) = \sum_i \nu i (H°_{298} - H°_0)i$$

where the sum of enthalpy increments $(H°_{298} - H°_0)$ is taken over all the i products and reactants, with the number of moles of each given by νi, where νi is positive for the products and negative for the reactants. The quantity $\Delta Hf°(\text{at } T)$ is also frequently given at a series of temperatures.

21.4 Calculation of Thermochemical Quantities

21.4.1 Additivity of Chemical Processes

Any chemical process can be conceived as occurring in stages, for each of which a chemical reaction can be written. These processes are additive in effect, and the overall re-action is the sum of the reactions into which it has been

resolved. As an example, we give the combustion of carbon to form carbon monoxide (equation 21.1) followed by the combustion of carbon monoxide to form carbon dioxide (equation 21.2). Energies are in kcal mol^{-1}.

$$C(graphite) + \tfrac{1}{2}O_2(g) \rightarrow CO(g) \qquad \Delta H^\circ_{298} = -26.416 \qquad (21.1)$$

$$CO(g) + \tfrac{1}{2}O_2(g) \rightarrow CO_2(g) \qquad \Delta H^\circ_{298} = -67.635 \qquad (21.2)$$

$$C(graphite) + O_2(g) \rightarrow CO_2(g) \qquad \Delta H^\circ_{298} = -94.051 \qquad (21.3)$$

The sum of the reactions is the appropriate reaction for the complete combustion of carbon directly to form carbon dioxide (equation 21.3). In summing such a sequence of reactions the same substance is not ordinarily shown on both sides of the final reaction, but only the excess on one side or the other.

As another illustration we give the combustion of an organic substance (for example, cellulose for which the repeating unit is $C_6H_{10}O_5$) to form carbon dioxide and gaseous water (equation 21.4), followed by condensation of the water to liquid (equation 21.5). The overall reaction may be written as the combustion of the organic substance to form gaseous carbon dioxide and liquid water (equation 21.6).

$$C_6H_{10}O_5(solid) + 6O_2(g) \rightarrow 6CO_2(g) + 5H_2O(g) \qquad (21.4)$$

$$5H_2O(g) \rightarrow 5H_2O(liq) \qquad (21.5)$$

$$C_6H_{10}O_5(solid) + 6O_2(g) \rightarrow 6CO_2(g) + 5H_2O(liq) \qquad (21.6)$$
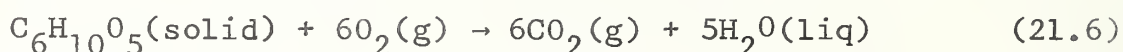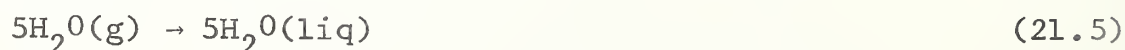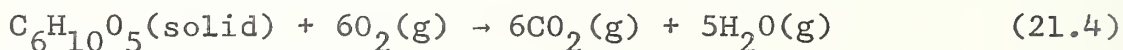
21.4.2 <u>Additivity of Thermodynamic Quantities (Law of Hess)</u>

When a sequence of chemical processes is carried out, as illustrated in Section 21.4.1, the thermodynamic quantities associated with the reaction are additive in the same way as the chemical reactions. The overall thermodynamic change of the final process is the sum of the thermodynamic changes of the intermediate or postulated processes into which it has been resolved.

Changes of enthalpy, internal energy, Gibbs energy, Helmholtz energy, and entropy are additive in this way. The enthalpy changes associated with reactions (21.1), (21.2), and (21.3) are given beside the equations for illustration. A sequence of processes of any desired length can be added this way.

21.5   Enthalpy and Internal Energy of Combustion

21.5.1   Calculation of Observed Heat Effects from Enthalpies of Formation

Combustion processes can be carried out practically in a variety of ways. Commercially, for example, combustion is often carried out as a flowing, nearly adiabatic process operated at constant pressure. The heat of reaction is dissipated through insulated walls, to heat exchange surfaces, and in heating quench water, or is carried up the stack in the products of combustion. Adiabatic constant-volume calculations are also useful in a practical way to determine pressure and temperature build-up from explosive combustions which might occur in incinerators.

In order to calculate the enthalpy of combustion (ΔHc) or internal energy of combustion (ΔUc) of a substance, it is essential to know the products of combustion and their proportions. The products and their proportions depend, first of all, on the composition of the substances burned and the oxidizer used. In addition, however, they depend upon the conditions of the combustion process. Factors involved include the pressure of the oxidizing air, the temperature and pressure reached by the reacting system, the relative proportions of elements present, and the rates at which substances pass through various reaction zones.

In this space it is impossible to give a complete analysis of the factors involved and methods for making calculations. However, the processes involved can be resolved into idealized simpler processes; the

isothermal process and the adiabatic process. A brief discussion of some of the factors involved in adiabatic processes and other processes, in which the reaction products are hot, is given in Sections 21.6 and 21.7. In the following two sections (21.5.2 and 21.5.3) we limit ourselves to enthalpy and internal energy changes and the related heat effects for some isothermal processes representing the combustion of substances as determined under idealized conditions. In Section 21.5.4 we extend the discussion to the combustion of several types of organic compounds, and in Section 21.5.5 discuss some other formalized fuel combustion reactions. We shall restrict our discussion to combustion in which oxygen (or air) is the oxidizer.

The isothermal process is a convenient form for presenting carefully defined thermodynamic information in a standard way, in which the heat observed can be expressed in terms of enthalpies of formation listed in tables of this handbook. Isothermal combustion can be carried out at constant pressure or at constant volume. These two processes are discussed below.

21.5.2 Isothermal Constant-Pressure Combustion

Combustion can be carried out in an open burner as a constant-pressure process with all reactants and products at the same initial and final temperature and pressure. The heat effect observed, $Q_p(obs)$, in which the subscript p represents the constant-pressure process is a measure of the enthalpy change.

In a constant-pressure process, typically though not necessarily, water and any other appreciably volatile substance among the products

remain in the gas phase, and oxygen is present in excess. In this case the observed heat effect which we shall calculate is closely related but not identical to the quantity, net heat of combustion, used in fuel technology (See Section 21.5.6).

For the purpose of this illustration we shall presume that ΔH and $\Delta H°$ do not differ significantly. Hence we may write:

$$Qp(obs) = -\Delta Hc(at\ T\ K) \approx -\Delta Hc°(at\ T\ K)$$

For a typical reaction, the combustion of polyethylene, equation (21.7) represents the process per mole of monomer unit.

$$C_2H_4(solid\ polymer) + 3O_2(g) \rightarrow 2CO_2(g) + 2H_2O(g) \qquad (21.7)$$
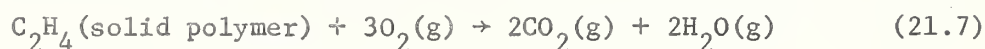
The enthalpy change for reaction (21.7) can be calculated from data in Tables I, II, and III.

$$\Delta Hc°(at\ 298\ K) = 2\Delta Hf°[CO_2(g)] + 2\Delta Hf°[H_2O(g)] - \Delta Hf[C_2H_4(solid\ polymer)]$$

$$= 2(-393.509) + 2(-241.818) - (-56.48)\ kJ\ mol^{-1}$$

$$= -1214.17\ kJ\ mol^{-1}$$

$$Qp(obs) \approx \Delta Hc(at\ 298\ K) = -1214.17\ kJ\ mol^{-1}$$

As the molecular weight of polyethylene (monomer unit) is 28.0542 g (0.0280542 kg) the specific net heat of combustion of polyethylene is $\frac{-1214.17}{28.0542} = -43.28$ MJ/kg.

During the reaction an increase in volume occurs, representing principally the increase in number of moles of gas, Δn. The increase in the amount of gas is 1 mole of gas per mole of reactant (4 moles of gas formed minus 3 moles of gas reacted). On the basis that the volume of

solid reactant is small compared to the increase in volume of the gases, and that the gases follow the ideal gas law, the work term $p\,\Delta V$ is expressible as

$$p\,\Delta V \simeq \Delta nRT$$

At 298.15 K, RT has the value 2.479 kJ mol^{-1}. As $\Delta n = 1$, $p\,\Delta V = 2.48$ kJ mol^{-1}.

If for any reason one wishes to calculate the internal energy change, $\Delta U°$(at 298 K) for reaction (21.7) it may now be done

$$
\begin{aligned}
\Delta U c°(\text{at } 298\ K) &= \Delta H c°(\text{at } 298\ K) - p\,\Delta V \\
&= -1214.17 - 2.48 \quad kJ\ mol^{-1} \\
&= -1216.65\ kJ\ mol^{-1} \\
&= -43.37\ MJ\ kg^{-1}
\end{aligned}
$$

21.5.3 Isothermal Constant-Volume Combustion

Combustion can be carried out in a closed burner as a constant-volume process with all reactants and products contained in the same volume and at the same temperature at beginning and end of the reaction. In a constant-volume process, it is customary to achieve complete combustion by using oxygen in excess and under a pressure of 20 to 30 atmospheres. In this case the heat effect, Qv, to which the subscript v has been added to represent the constant-volume process, is a measure of the internal energy change.

$$Qv(\text{obs}) = -\Delta U c \simeq \Delta U c°$$

If it is possible to devise a system in which all the products of reaction (21.7) remain in the gaseous state, then $-\Delta U c°$(at 298 K) would be as we have calculated it before and Qv(obs) would be 1216.65 kJ mol^{-1} (43.37 MJ kg^{-1}).

A more usual circumstance for a constant-volume process is for the condensable products of combustion to be condensed to the liquid state. In this case, the observed heat effect which we shall calculate is closely related, though not identical, to the gross heat of combustion (see Section 21.5.6) used in fuel technology. In this case, the observed reaction would be given by equation (21.8).

$$C_2H_4(\text{solid polymer}) + 3O_2(g) \rightarrow 2CO_2(g) + 2H_2O(\text{liq}) \qquad (21.8)$$

The enthalpy change again can be computed using data from Tables I, II, and III

$$
\begin{aligned}
\Delta H^\circ(\text{at } 298 \text{ K}) &= 2\,\Delta H f^\circ[CO_2(g)] + 2\,\Delta H f^\circ[H_2O(\text{liq})] - \Delta H f^\circ[C_2H_4(\text{solid polymer})] \\
&= 2(-393.509) + 2(-285.830) - (-56.99) \text{ kJ mol}^{-1} \\
&= -1302.20 \text{ kJ mol}^{-1} \\
&= -46.42 \text{ MJ kg}^{-1}
\end{aligned}
$$

As before, we can now calculate the internal energy change. In this case, because the water was condensed, the number of moles of gas is reduced; $\Delta n = -1$ mole per mole of reactant.

$$
\begin{aligned}
p\,\Delta V &\approx \Delta n\, RT = -2.48 \text{ kJ mol}^{-1} \\
\Delta U c^\circ(\text{at } 298 \text{ K}) &= \Delta H c^\circ(\text{at } 298 \text{ K}) - p\,\Delta V \\
&= -1302.20 - (-2.48) \text{ kJ mol}^{-1} \\
&= -1299.72 \text{ kJ mol}^{-1} \\
&= -46.33 \text{ MJ kg}^{-1}
\end{aligned}
$$

Thus for this constant volume process

$$
\begin{aligned}
Q_v(\text{obs}) &\approx -\Delta U^\circ(\text{at } 298 \text{ K}) = 1299.72 \text{ kJ mol}^{-1} \\
&= 46.33 \text{ MJ kg}^{-1}
\end{aligned}
$$

Note that both $\Delta Uc°$(at 298 K) and $\Delta Hc°$(at 298 K) are more negative for reaction (21.8) than the corresponding values for reaction (21.7), and the reaction is, therefore, more exothermic. The extra heat comes from the condensation of the water.

21.5.4 Type Reactions for Combustion of Organic Compounds- Calculation of Enthalpy of Combustion for the Isothermal Process

The substances present in the combustion products depend first upon the elements present. The phases of the products (gas, liquid, or solid) depend upon the temperatures and partial pressures of the substances at the conclusion of the process.

Calculations of ΔUc or ΔHc(at 298 K) such as are shown in the preceding section can be made for any given process, provided the equation can be written for the process, and provided the enthalpies of formation of reactants and products are known.

To assist in the calculation of the energy changes, equations are given in Table 21.1 and Table 21.3 for a standard type reaction for each of several classes of organic compounds.

The classes of compounds are based on the elements present in an empirical formula, and are not functional classes. Compound classes containing various typical combinations of the elements C, H, N, O, P, S, F, Cl, Br, and I are given. Not all possible combinations are given. However, the pattern of the reactions should be clear from the table, and it should be possible for the user to extend the table to include all the information required for other combinations of the same elements.

The products of combustion that will be encountered are different, depending upon whether the process is carried out at constant volume or at constant pressure, and the product in which a given element is found depends to some extent upon other elements present.

For the combustion processes, we make the following somewhat arbitrary presumptions. Some water will have been supplied in the constant-volume process to dissolve the soluble acids formed.

The product of combustion of carbon is $CO_2(g)$.

The product of combustion of hydrogen is $H_2O(g)$ in the constant-pressure process, and $H_2O(liq)$ in the constant-volume process. If the halogens F or Cl are present, some of the hydrogen may be present as $HF(g)$ or $HCl(g)$ in the constant-pressure process in which water is formed as a gas, or as $HF(aq)$ or $HCl(aq)$ in the constant-volume process in which condensables are condensed. If sulfur or phosphorus is present, some of the hydrogen may be present as $H_2SO_4(aq)$ or $H_3PO_4(aq)$ in the constant-volume process, in which water and other condensables have condensed.

The product of combustion of organic nitrogen is taken to be the gaseous element, $N_2(g)$. Some oxides of nitrogen may be formed in the constant-pressure process, and some $HNO_3(aq)$ may be formed in the constant-volume process. A correction to the enthalpy change of the type process may be required, to obtain the observed heat, if appreciable quantities of either are formed. Some oxides of nitrogen or nitric acid may also be formed, even if the element is absent in the combustible substance, because nitrogen from the combustion air may combine with

oxygen at the temperature and pressure of the combustion reaction. The occurrence of nitrogen-oxygen compounds may be expected to be much more pronounced in the constant-volume process than in the constant-pressure process, because of the higher temperatures usually reached in the constant-volume process, and possibly also because of the reduction in number of moles of gas caused by formation of the compounds.

The product of combustion of organic phosphorus is taken here to be $P_4O_{10}(g)$ in the constant-pressure process and $H_3PO_4(aq)$ in the constant-volume process. The presumed concentration of H_3PO_4 is one mole in 40 moles of H_2O. If the resulting concentration in an actual combustion differs appreciably from this, a dilution correction may be required in order to calculate Qv(obs). Note that some compilations of enthalpies of combustion of phosphorus compounds presume the final form of the phosphorus to be $H_3PO_4(c)$, and hence care must be taken when comparing enthalpies of combustion from various sources.

The product of combustion of organic sulfur is taken to be $SO_2(g)$ in the constant-pressure process and $H_2SO_4(aq)$ in the constant-volume process. The conversion to the higher oxidation state is catalyzed by oxides of nitrogen, and the conversion may be expected to be nearly complete if appreciably high pressures and temperatures are developed. The presumed concentration of H_2SO_4 is one mole in 115 moles of H_2O. If the resulting concentration in an actual combustion differs appreciably from this, a dilution correction may be required in order to calculate Qv(obs).

The product of combustion of organic fluorine is taken to be HF(g) in the constant-pressure process, and HF(aq) in the constant-volume process. The presumed concentration of HF is one mole in 20 moles of H_2O. If the resulting concentration in an actual combustion differs from this by an appreciable amount, a dilution correction may be required in order to calculate Qv(obs). The formation of HF by burning an organic compound in oxygen depends upon the presence of hydrogen in the combustion material. If hydrogen is not present in sufficient quantity to combine with all the fluorine, the balance of the fluorine will appear as CF_4, or possibly COF_2, unless other elements (such as metals) are present. If not wanted, this contingency can be avoided by adding an auxiliary combustible which contains enough hydrogen to combine with the fluorine. The equation for this alternate process is given (Equation 9, Table 21.3). If CF_4 or COF_2 are formed and their avoidance is not deemed necessary, the calculation of Qv(obs) will be affected by the proportions present, which may be determined by analysis or by calculation from equilibria.

The product of combustion of organic chlorine is taken to be HCl(g) in the constant-pressure process, and HCl(aq) in the constant-volume process. The presumed concentration of HCl is one mole of HCl in 600 moles of H_2O. If the resulting concentration differs appreciably from this, a dilution correction may be required in order to calculate Qv(obs) accurately. Because oxygen and chlorine are of comparable electronegativity, the possibility of forming elemental chlorine, Cl_2(g), exists. If its presence is objectionable, it may be possible to remove it by use of a reducing agent, such as As_2O_3(aq), outside the combustion

zone. A correction must be applied to Qv(obs) for the reduction process.
If the presence of Cl_2(g) must be allowed, the calculation of Qv(obs) is
affected, and the proportions of Cl_2 and HCl may have to be determined
by analysis or from equilibrium calculations in order to determine Qv(obs).
Experience indicates that 15 to 20% of the chlorine is formed as Cl_2 and
80 to 85% as HCl in the constant-volume process.

The product of combustion of organic bromine is taken to be
elemental bromine, as the gas in the constant-pressure process and as
the liquid in the constant-volume process. The form of the bromine in
a given reaction system should be determined by analysis. In calculating
Qv(obs) or Qp(obs), a correction can be applied to ΔU or ΔH for any
deviation from the equation given. Experience indicates that 90 to 97%
of the bromine is formed as Br_2(liq) in the constant-volume process.

The product of combustion of organic iodine is taken to be
elemental iodine, as the gas in the constant-pressure process. For a
given reaction system, the form of the iodine should be determined by
actual analysis. In calculating Qv(obs) or Qp(obs) a correction can
be applied to ΔU or ΔH for any deviation from the equation.

Table 21.1 presents type equations for combustion reactions of
organic compounds burning at constant pressure in an atmosphere of
oxygen. The equations are balanced with generalized letter coefficients
derived from the letter subscripts of the elements in the formula. The
stoichiometric amount of oxygen and the amounts of the type reaction
products are given. Table 21.1 is supplemented by Table 21.2 which
gives for the reactions the elements present, the increase in quantity
of gas, Δn, calculated from the amounts of gaseous products and reactants

Table 21.1

Type Combustion Reactions of Organic Compounds Burning at Constant Pressure in an Atmosphere of Oxygen

All Products Emitted as Gases

	Substance(*)		Stoichiometric oxygen		Products
(1)	C_aH_b(c,liq)	+	$(a + \frac{b}{4})$ O_2(g)	→	a CO_2(g) + $\frac{b}{2}$ H_2O(g)
(2)	$C_aH_bN_c$(c,liq)	+	$(a + \frac{b}{4})$ O_2(g)	→	a CO_2(g) + $\frac{b}{2}$ H_2O(g) + $\frac{c}{2}$ N_2(g)
(3)	$C_aH_bO_d$(c,liq)	+	$(a + \frac{b}{4} - \frac{d}{2})$ O_2(g)	→	a CO_2(g) + $\frac{b}{2}$ H_2O(g)
(4)	$C_aH_bN_cO_d$(c,liq)	+	$(a + \frac{b}{4} - \frac{d}{2})$ O_2(g)	→	a CO_2(g) + $\frac{b}{2}$ H_2O(g) + $\frac{c}{2}$ N_2(g)
(5)	$C_aH_bO_dP_e$(c,liq)	+	$(a + \frac{b}{4} - \frac{d}{2} + \frac{5}{4}e)$ O_2(g)	→	a CO_2(g) + $\frac{b}{2}$ H_2O(g) + $\frac{e}{4}$ P_4O_{10}(g)
(6)	$C_aH_bO_dS_f$(c,liq)	+	$(a + \frac{b}{4} - \frac{d}{2} + f)$ O_2(g)	→	a CO_2(g) + $\frac{b}{2}$ H_2O(g) + f SO_2(g)
(7)	$C_aH_bN_cO_dS_f$(c,liq)	+	$(a + \frac{b}{4} - \frac{d}{2} + f)$ O_2(g)	→	a CO_2(g) + $\frac{b}{2}$ H_2O(g) + $\frac{c}{2}$ N_2(g) + f SO_2(g)
(8)	$C_aH_bF_g$(c,liq)	+	$(a + \frac{b}{4} - \frac{g}{4})$ O_2(g)	→	a CO_2(g) + $(\frac{b}{2} - \frac{g}{2})$ H_2O(g) + g HF(g)
(9)	$C_aH_bF_g$(c,liq) + x $C_{a'}H_{b'}$(c,liq)	+	$(a + x a' + \frac{b}{4} + \frac{x b'}{4} - \frac{g}{4})$ O_2(g)	→	$(a + x a')$ CO_2(g) + $(\frac{b}{2} + \frac{x b'}{2} - \frac{g}{2})$ H_2O(g) + g HF(g)
(10)	$C_aH_bCl_h$(c,liq)	+	$(a + \frac{b}{4} - \frac{h}{4})$ O_2(g)	→	a CO_2(g) + $(\frac{b}{2} - \frac{h}{2})$ H_2O(g) + h HCl(g)
(11)	$C_aH_bBr_i$(c,liq)	+	$(a + \frac{b}{4})$ O_2(g)	→	a CO_2(g) + $\frac{b}{2}$ H_2O(g) + $\frac{i}{2}$ Br_2(g)
(12)	$C_aH_bI_j$(c,liq)	+	$(a + \frac{b}{4})$ O_2(g)	→	a CO_2(g) + $\frac{b}{2}$ H_2O(g) + $\frac{j}{2}$ I_2(g)

(*) (c,liq) indicates that the equations are valid for either solid or liquid substance

(g) indicates that the equations are valid for gaseous substance.

Table 21.2, Enthalpy Changes for Table 21.1

Reaction	Elements	Δn^*	$p\Delta V = \Delta n\,RT = 0.592\,\Delta n$ ΔH° (at 298 K), kcal mol^{-1}	$p\Delta V = \Delta n\,RT = 2.477\,\Delta n$ ΔH° (at 298 K), kJ mol^{-1}
(1)	C,H	$(\frac{b}{4})$	$-94.051a -57.796\frac{b}{2} -\Delta Hf[\text{substance}]$	$-393.51a -241.82\frac{b}{2} -\Delta Hf[\text{substance}]$
(2)	C,H,N	$(\frac{b}{4} + \frac{c}{2})$	$-94.051a -57.796\frac{b}{2} -\Delta Hf[\text{substance}]$	$-393.51a -241.82\frac{b}{2} -\Delta Hf[\text{substance}]$
(3)	C,H,O	$(\frac{b}{4} + \frac{d}{2})$	$-94.051a -57.796\frac{b}{2} -\Delta Hf[\text{substance}]$	$-393.51a -241.82\frac{b}{2} -\Delta Hf[\text{substance}]$
(4)	C,H,N,O	$(\frac{b}{4} + \frac{c}{2} + \frac{d}{2})$	$-94.051a -57.796\frac{b}{2} -\Delta Hf[\text{substance}]$	$-393.51a -241.82\frac{b}{2} -\Delta Hf[\text{substance}]$
(5)	C,H,O,P	$(\frac{b}{4} + \frac{d}{2} - e)$	$-94.051a -57.796\frac{b}{2} -677.4\frac{e}{4} -\Delta Hf[\text{substance}]$	$-393.51a -241.82\frac{b}{2} -2834.2\frac{e}{4} -\Delta Hf[\text{substance}]$
(6)	C,H,O,S	$(\frac{b}{4} + \frac{d}{2})$	$-94.051a -57.796\frac{b}{2} -70.94f -\Delta Hf[\text{substance}]$	$-393.51a -241.82\frac{b}{2} -296.83f -\Delta Hf[\text{substance}]$
(7)	C,H,N,O,S	$(\frac{b}{4} + \frac{c}{2} + \frac{d}{2})$	$-94.051a -57.796\frac{b}{2} -70.94f -\Delta Hf[\text{substance}]$	$-393.51a -241.82\frac{b}{2} -296.83f -\Delta Hf[\text{substance}]$
(8)	C,H,F	$(\frac{b}{4} + \frac{3g}{4})$	$-94.051a -57.796(\frac{b}{2} - \frac{g}{2}) -65.15g -\Delta Hf[\text{substance}]$	$-393.51a -241.82(\frac{b}{2} - \frac{g}{2}) -272.55g -\Delta Hf[\text{substance}]$
(9)	C,H,F,	$(\frac{b}{4} + \frac{x\acute{b}}{4} + \frac{3g}{4})$	$-94.051(a + x\acute{a}) -57.796(\frac{b}{2} + \frac{x\acute{b}}{2} - \frac{g}{2}) -65.14g -\Delta Hf[\text{substance}] -xHf[\text{auxiliary}]$	$-393.51(a + x\acute{a}) -241.82(\frac{b}{2} + \frac{x\acute{b}}{2} - \frac{g}{2}) -272.59g -\Delta Hf[\text{substance}] -xHf[\text{auxiliary}]$
(10)	C,H,Cl	$(\frac{b}{4} + \frac{3h}{4})$	$-94.051a -57.796(\frac{b}{2} - \frac{h}{2}) -22.06h -\Delta Hf[\text{substance}]$	$-393.51a -241.82(\frac{b}{2} - \frac{h}{2}) -92.31h -\Delta Hf[\text{substance}]$
(11)	C,H,Br	$(\frac{b}{4} - \frac{i}{2})$	$-94.051a -57.796\frac{b}{2} +7.39\frac{i}{2} -\Delta Hf[\text{substance}]$	$-393.51a -241.82\frac{b}{2} +30.91\frac{i}{2} -\Delta Hf[\text{substance}]$
(12)	C,H,I	$(\frac{b}{4} + \frac{i}{2})$	$-94.051a -57.796\frac{b}{2} +14.92\frac{i}{2} -\Delta Hf[\text{substance}]$	$-393.51a -241.82\frac{b}{2} +62.44\frac{i}{2} -\Delta Hf[\text{substance}]$

*Δn is the increase in number of moles of gas when the combustible material is not a gas. Under some circumstances Δn may be negative.

$p\Delta V = \Delta n\,RT$ on the basis that (a) the gases are ideal, and (b) the volume of the condensed phase can be neglected in comparison with change in volume of gas.

Table 21.3 Type Combustion Reactions of Organic Compounds Burning at Constant Volume in an Atmosphere of Oxygen (Excess Water Present)

Products are Formed as Gases and Aqueous Solutions

	Substance	Stoichiometric Oxygen	Products
(1)	C_aH_b(c,liq)	$+ \left(a + \frac{b}{4}\right) O_2(g)$	$\rightarrow$ $a\,CO_2(g) + \frac{b}{2} H_2O(liq)$
(2)	$C_aH_bN_c$(c,liq)	$+ \left(a + \frac{b}{4}\right) O_2(g)$	$\rightarrow$ $a\,CO_2(g) + \frac{b}{2} H_2O(liq) + \frac{c}{2} N_2(g)$
(3)	$C_aH_bO_d$(c,liq)	$+ \left(a + \frac{b}{4} - \frac{d}{2}\right) O_2(g)$	$\rightarrow$ $a\,CO_2(g) + \frac{b}{2} H_2O(liq)$
(4)	$C_aH_bN_cO_d$(c,liq)	$+ \left(a + \frac{b}{4} - \frac{d}{2}\right) O_2(g)$	$\rightarrow$ $a\,CO_2(g) + \frac{b}{2} H_2O(liq) + \frac{c}{2} N_2(g)$
(5)	$C_aH_bO_dP_e$(c,liq)	$+ \left(a + \frac{b}{4} - \frac{d}{2} + \frac{5}{4}e\right) O_2(g)$	$\rightarrow$ $a\,CO_2(g) + \left(\frac{b}{2} - \frac{3e}{2}\right) H_2O(liq) + e\,H_3PO_4$ (aq in 40 H_2O)
(6)	$C_aH_bO_dS_f$(c,liq)	$+ \left(a + \frac{b}{4} - \frac{d}{2} + \frac{3f}{2}\right) O_2(g)$	$\rightarrow$ $a\,CO_2(g) + \left(\frac{b}{2} - f\right) H_2O(liq) + f\,H_2SO_4$ (aq in 115 H_2O)
(7)	$C_aH_bN_cO_dS_f$(c,liq)	$+ \left(a + \frac{b}{4} - \frac{d}{2} + \frac{3f}{2}\right) O_2(g)$	$\rightarrow$ $a\,CO_2(g) + \left(\frac{b}{2} - f\right) H_2O(liq) + \frac{c}{2} N_2(g) + f\,H_2SO_4$ (aq in 115 H_2O)
(8)	$C_aH_bF_g$(c,liq)	$+ \left(a + \frac{b}{4} - \frac{g}{4}\right) O_2(g)$	$\rightarrow$ $a\,CO_2(g) + \left(\frac{b}{2} - \frac{g}{2}\right) H_2O(liq) + g\,HF$(aq in 20 H_2O)
(9)	$C_aH_bF_g$(c,liq) $+ xC_{a'}H_{b'}$(c,liq)	$+ \left(a + xa' + \frac{b}{4} + \frac{xb'}{4} - \frac{g}{4}\right) O_2(g)$	$\rightarrow$ $(a + xa')\,CO_2(g) + \left(\frac{b}{2} + \frac{xb'}{2} - \frac{g}{2}\right) H_2O(liq) + g\,HF$(aq in 20 H_2O)
(10)	$C_aH_bCl_h$(c,liq)	$+ \left(a + \frac{b}{4} - \frac{h}{4}\right) O_2(g)$	$\rightarrow$ $a\,CO_2(g) + \left(\frac{b}{2} - \frac{h}{2}\right) H_2O(liq) + h\,HCl$ (aq in 600 H_2O)
(11)	$C_aH_bBr_i$(c,liq)	$+ \left(a + \frac{b}{4}\right) O_2(g)$	$\rightarrow$ $a\,CO_2(g) + \frac{b}{2} H_2O(liq) + \frac{i}{2} Br_2(liq)$
(12)	$C_aH_bI_j$(c,liq)	$+ \left(a + \frac{b}{4}\right) O_2(g)$	$\rightarrow$ $a\,CO_2(g) + \frac{b}{2} H_2O(liq) + \frac{j}{2} I_2(c)$

Table 21.4 Enthalpy Changes for Table 21.3

Reaction	Elements	Δn*	$p\Delta V \approx \Delta nRT = 0.592\ \Delta n$ $\Delta H°$ (at 298 K), kcal mol^{-1}	$p\Delta V \approx \Delta nRT = 2.477\ \Delta n$ $\Delta H°$ (at 298 K), kJ mol^{-1}
(1)	C,H	$\left(-\dfrac{b}{4}\right)$	$-94.051a - \dfrac{b}{2} - \Delta Hf[\text{substance}]$	$-393.51a - 285.83\dfrac{b}{2} - \Delta Hf[\text{substance}]$
(2)	C,H,N	$\left(\dfrac{c}{2} - \dfrac{b}{4}\right)$	$-94.051a - \dfrac{b}{2} - \Delta Hf[\text{substance}]$	$-393.51a - 285.83\dfrac{b}{2} - \Delta Hf[\text{substance}]$
(3)	C,H,O	$\left(\dfrac{d}{2} - \dfrac{b}{4}\right)$	$-94.051a - 68.315\dfrac{b}{2} - \Delta Hf[\text{substance}]$	$-393.51a - 285.83\dfrac{b}{2} - \Delta Hf[\text{substance}]$
(4)	C,H,N,O	$\left(\dfrac{c}{2} - \dfrac{d}{2} - \dfrac{b}{4}\right)$	$-94.051a - 68.315\dfrac{b}{2} - \Delta Hf[\text{substance}]$	$-393.51a - 285.83\dfrac{b}{2} - \Delta Hf[\text{substance}]$
(5)	C,H,O,P	$\left(\dfrac{d}{2} - \dfrac{b}{4}\right)$	$-94.051a - 68.315\left(\dfrac{b}{2} - \dfrac{3e}{2}\right) - 308.032e$	$-393.51a - 285.83\left(\dfrac{b}{2} - \dfrac{3e}{2}\right) - 1288.81e$
(6)	C,H,O,S	$\left(\dfrac{d}{2} - \dfrac{b}{4} - \dfrac{3f}{2}\right)$	$-94.051a - 68.315\left(\dfrac{b}{2} - \dfrac{f}{2}\right) - 212.192f$ $-\Delta Hf[\text{substance}]$	$-393.51a - 285.83\left(\dfrac{b}{2} - \dfrac{f}{2}\right) - 887.81f$ $-\Delta Hf[\text{substance}]$
(7)	C,H,N,O,S	$\left(\dfrac{c}{2} + \dfrac{d}{2} - \dfrac{b}{4} - \dfrac{3f}{2}\right)$	$-94.051a - 68.315\left(\dfrac{b}{2} - \dfrac{f}{2}\right) - 212.192f$ $-\Delta Hf[\text{substance}]$	$-393.51a - 285.83\left(\dfrac{b}{2} - \dfrac{f}{2}\right) - 887.81f$ $-\Delta Hf[\text{substance}]$
(8)	C,H,F	$\left(\dfrac{g}{4} - \dfrac{b}{4}\right)$	$-94.051a - 68.315\left(\dfrac{b}{2} - \dfrac{g}{2}\right) - 76.71g$ $-\Delta Hf[\text{substance}]$	$-393.51a = 285.83\left(\dfrac{b}{2} - \dfrac{g}{2}\right) - 320.95g$ $-\Delta Hf[\text{substance}]$
(9)	C,H,Cl	$\left(\dfrac{g}{4} - \dfrac{b}{4} - \dfrac{x\acute{b}}{4}\right)$	$-94.051(a + x\acute{a}) - 68.315\left(\dfrac{b}{2} + \dfrac{xb}{2} - \dfrac{g}{2}\right)$ $-76.71g - \Delta Hf[\text{substance}]$	$-393.51(a + x\acute{a}) - 285.83\left(\dfrac{b}{2} + \dfrac{xb}{2} - \dfrac{g}{2}\right)$ $-320.95g - \Delta Hf[\text{substance}]$
(10)	C,H,Cl	$\left(\dfrac{h}{4} - \dfrac{b}{4}\right)$	$-94.051a - 68.315\left(\dfrac{b}{2} - \dfrac{h}{2}\right) - 39.823h$ $-\Delta Hf[\text{substance}]$	$-393.51a - 285.83\left(\dfrac{b}{2} - \dfrac{h}{2}\right) - 166.62h$ $-\Delta Hf[\text{substance}]$
(11)	C,H,Br	$\left(-\dfrac{b}{4}\right)$	$-94.051a - 68.315\dfrac{b}{2} - \Delta Hf[\text{substance}]$	$-393.51a - 285.83\dfrac{b}{2} - \Delta Hf[\text{substance}]$
(12)	C,H,I	$\left(-\dfrac{b}{4}\right)$	$-94.051a - 68.315\dfrac{b}{2} - \Delta Hf[\text{substance}]$	$-393.51a - 285.83\dfrac{b}{2} - \Delta Hf[\text{substance}]$

* See footnote Table 21.2

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Table 21.5 Auxiliary Data for Determining Enthalpies
of Combustion of Organic Compounds

Substance (state)	$\Delta Hf°$ kcal mol^{-1}	$\Delta Hf°$ kJ mol^{-1}	Reference
CO_2(g)	−94.051	−393.51	[1]
H_2O(g)	−57.796	−241.82	[1]
H_2O(liq)	−68.315	−285.83	[1]
HF(g)	−65.14	−272.55	[2]
HF(aq) (20 H_2O)	−76.71	−320.95	[3]
HCl(g)	−22.062	−92.31	[1]
HCl(aq) (600 H_2O)	−39.823	−166.62	[1]
HBr(g)	−8.70	−36.40	[1]
HBr(aq) (600 H_2O)	−28.935	−121.06	[1]
HI(g)	+6.33	+26.48	[1]
HI(aq) (600 H_2O)	−13.088	−54.76	[1]
H_3PO_4 (40 H_2O)	−308.032	−1288.81	[1]
P_4O_{10}(g)	−677.4	−2834.2	[2]
SO_2(g)	−70.944	−296.83	[1]
H_2SO_4(115 H_2O)	−212.192	−887.81	[1]
Br_2(g)	+7.387	+30.91	[1]
I_2(g)	+14.923	+62.44	[1]
I_2(c)	0.0	0.0	[1]
Br_2(liq)	0.0	0.0	[1]

[1] Wagman, D. D., Evans, W.H., Parker, V. B., Harlow, I., Bailey, S. M., and Schumm, R. H., Nat. Bur. Standards Technical Note 270-3, January 1968.

[2] Stull, D. R., and Prophet, H., JANAF Thermochemical Tables, 2nd Edition, National Standard Reference Data System, NSRDS-NBS-37, 1141 pp. (June 1971) (U.S. Government Printing Office, Washington, D. C. 20402).

[3] Domalski, E. S. and Armstrong, G. T., J. Research NBS 71A, 105–118 (1967).

determined from the stoichiometry, and expressions for calculating $\Delta H°$ (at 298 K) in kcal mol^{-1} and kJ mol^{-1} from the enthalpies of formation of products and reactants given in Tables I, II, and III and Table 21.5.

Table 21.3 presents type reactions for combustion reactions of organic compounds burning at constant volume in an atmosphere of oxygen, with water added to dissolve product acids, and all water formed condensed to the liquid state. In other respects Tables 21.3 and 21.4 are similar to Tables 21.1 and 21.2, respectively.

Table 21.5 gives the values of $\Delta Hf°$ (at 298 K) in kcal mol^{-1} and in kJ mol^{-1} for products found in Tables 21.1 and 21.3 These data were used in deriving the equations of Tables 21.2 and 21.4. They can be used to calculate the enthalpy and internal energy changes for combustion of particular substances, and for other reactions, following the procedures described in this and the preceding sections.

21.5.5 Enthalpies of Formation by Estimation

Supplementary sources of enthalpies of formation, many of which are not found in Tables I, II, or III may be found in monographs listed in Section 22.0.

If the value of the enthalpy of formation (or enthalpy of combustion) is not found in any available reference source, it is possible to estimate a value which is reasonably accurate. Monographs, chapters of books, and review articles giving methods for estimating various thermodynamic quantities are given in Section 23.0. Values of enthalpies of formation estimated using these methods may be in error by one to five kcal mol^{-1} (4 to 20 kJ mol^{-1}).

21.5.6 <u>Calorific Values or Heating Values of Fuels</u>

The terminology of heating values used in the fuel industries
and applied to coal, coke, petroleum products, and natural or manu-
factured gas, refers to quantities closely related to the enthalpy
and internal energy of combustion as discussed in this book. The terms
given below may be found in use. The following definitions are quoted
from ASTM methods referenced.

<u>Standard Definition of the Terms Gross Calorific Value and Net</u>
<u>Calorific Value of Solid and Liquid Fuels</u> (Definitions (1) and (2) are
found in Reference (1) below).

(1) <u>gross calorific value (gross heat of combustion)</u>, Qg in the
case of solid fuels and liquid fuels of low volatility, the heat produced
by combustion of unit quantity, at constant volume, in an oxygen bomb
calorimeter, under specified conditions.
Note - The conditions are initial oxygen pressure of 20 to 40 atm, final
temperature of 68 to 95 F (20 to 35 C), products in form of ash, liquid
water, and gaseous CO_2, SO_2, and nitrogen. This definition is not applied
to gaseous or highly volatile liquid fuels.

(2) <u>net calorific value, (net heat of combustion)</u>, Qn in the case
of solid fuels and liquid fuels of low volatility, a lower value calculated
from the gross calorific value as the heat produced by combustion of unit
quantity, at constant atmospheric pressure, under conditions such that all
water in the products remains in the form of vapor.
Note - The net calorific value (net heat of combustion) is calculated from
the gross calorific value (gross heat of combustion) at 68°F (20°C) by
making a deduction of 1030 Btu/lb. (572 cal/g) of water derived from unit

quantity of fuel, including both the water originally present as moisture

and that formed by combustion. The deduction is not equal to the latent

heat of vaporization of water (1055 Btu/lb. at 68 F (20 C) because the

calculation is made to reduce from gross value at constant volume to net

value at constant pressure, for which the appropriate factor under these

conditions is 1030 Btu/lb.

Definitions (1) and (2) are found in Reference (1) below. The quantities

Hi and Hs found in Reference (1) are respectively Qg and Qn above.

Slightly variant definitions can be found in other places. Also, in

different ASTM methods different base temperatures are found. The

quantities gross and net heat of combustion are therefore not very

explicitly defined.

For the conversion from gross to net heat of combustion, several

nearly equivalent formulas are found in the standard test literature.

These take into account the per cent hydrogen in the sample.

	Relation (at 25°C)			Units	ASTM Method	Fuel Type
(1)	Qn	= Qg	− 10.30(Hx9)	Btu/lb	D271-70;D2015-66	Coal, coke
(2)	Qn	= Qg	− 5.72(Hx9)	cal/g	D271-70	Coal, coke
(3)	Qp(net)	= Qv(gross)	− 91.23(H)	Btu/lb	D240-64;D2382-65	Petroleum Products
(4)	Qp(net)	= 0.7195 Qv(gross)	+ 4310	Btu/lb	D240-64;D2382-65	Petroleum Products

In the above equations H is per cent hydrogen by weight.

Qg is found referred to in the methods as Hs, Hg, Qg (gross at 25 C, or the

letters B and C.

Qn is found referred to in the methods as Hi, Hn or Qn (net at 25 C) or the

letters N and N'.

The terminology Qp (net, at 25°C) and Qv (gross, at 25°C) is due to
Jessup (Reference (3)). It uses Q for heat in a positive sense, uses
subscript p to indicate the constant pressure process and v to indicate
the constant volume process, and in parentheses states whether the net
or gross heating value is referred to and the temperature to which the
heat effect refers. It is a more explicit statement of the conditions
for which the heat effect is valid than are the other samples in use.

The slight discrepancy between formula (1) and formula (3)
should not be of concern. While formula (3) is probably based on a
more accurate analysis of the thermal effects involved, the inaccuracy
with which H is known and the variations from sample to sample in
measuring the heating value probably introduce larger uncertainties
than the differences.

To convert Qg to Qn the hydrogen content of the fuel must be
known. This is preferably determined by analysis. In the absence of
a measured value an estimate of the difference (Qg-Qn) for petroleum
fuels can be made. Equation (4) is a relationship based on an experi-
mental correlation between Qg and per cent hydrogen for liquid hydro-
carbons and hydrocarbon mixtures. It is not as accurate as equations
(1) or (3).

Equation (2) differs from equation (1) only in the factor
1.8 Btu/lb = 1.0 cal/g.

Definitions of Terms for Gaseous Fuels (Reference (1c), (1d) below).

(3) total calorific value, the total calorific value of a gas
is the number of British thermal units evolved by the complete combustion,
at constant pressure, of one standard cubic foot of gas with air, the

temperature of the gas, air, and products of combustion being 60°F, and
all the water formed by the combustion reaction being condensed to the
liquid state.

(4) net calorific value, the net calorific value of a gas is the
number of British thermal units evolved by the complete combustion, at
constant pressure, of one standard cubic foot of gas with air, the
temperature of the gas, air, and products of combustion being 60°F and
all of the water formed by the combustion reaction remaining in the
vapor state.

Note 1 - The net calorific value of a gas is its total calorific value
minus the latent heat of evaporation at standard temperature of the
water formed by the combustion reaction.

Note 2 - The definitions given [Terms (3) and (4)] are for total and net
calorific values per standard cubic foot of gas. The definitions corre-
sponding to any other unit quantity of gas are obtained by substituting
the name of the desired unit in place of the term "standard cubic foot"
in the definitions. Methods of calculating calorific values per cubic
foot of gas under any desired conditions of pressure, temperature, and
water vapor content are specified [in the ASTM method].

Definitions (3) and (4) are found in

ASTM Designation D900-55

Standard Method of Test for Calorific Value of Gaseous Fuels

by the Water Flow Calorimeter. See Reference (1) below.

Definition (3) is also found in:

ASTM Designation D1826-64

Standard Method of Test for Calorific Value of Gases in Natural

Gas Range by Continuous Recording Calorimeter. See Reference

(1) below.

The British thermal unit used in the gas industry and the standard

cubic foot of gas are also defined in these methods.

The gross heat of combustion at constant volume, Qv(gross) approximates $-\Delta U$, the change in internal energy of the combustion process with water formed in the liquid state. The negative sign appears because Qv(gross) is positive for an exothermic reaction, while ΔU is negative.

The net heat of combustion at constant pressure, Qp(net), approximates $-\Delta H$, the change in enthalpy of the combustion process with water formed in the gaseous state. The negative sign appears as above.

In ASTM Method D-2382 (See reference (2) below), the following caution is noted: Users of this method desiring to calculate ΔHc° at 298 K for a pure compound should note that corrections must be applied to the value of Qv(gross) for buoyancy of air, heat capacities of reaction components, reduction to a constant-pressure process, and deviation of the reaction from the thermodynamic standard state.

The total calorific value and the net calorific value of a gas differ only in that the water formed is condensed to determine the former and not the latter. Thus the value of the net heating value of a gas approximates the net heat of combustion at constant pressure but on a volumetric basis rather than a mass basis. The total calorific

value of a gas could be given the name gross heat of combustion at constant pressure, a term which is rarely if ever used.

References to Section 21.5

(1) 1971 Annual Book of ASTM Standards, Part 19. Gaseous Fuels; Coal and Coke. (American Society for Testing and Materials, Philadelphia, Pa., 19103).

  (a) D 271-70 Standard Method of Test for Analysis of Coal and Coke.

  (b) D 407-44 Standard Definitions of the Term Gross Calorific Value and Net Calorific Value of Solid and Liquid Fuels.

  (c) D 900-35 Standard Method of Test for Calorific Value of Gases by the Water Flow Calorimeter.

  (d) D 1826-64 Standard Method of Test for Calorific Value of Gases in Natural Gas Range by Continuous Recording Calorimeter.

  (e) D 2015-66 Standard Method of Test for Calorific Value by Adiabatic Bomb Calorimeter.

(2) 1971 Annual Book of ASTM Standards, Part 17, Petroleum Products-Fuels-Solvents; Burner Fuel Oils; Lubricating Oils; Cutting Oils; Lubricating Greases; Hydraulic Fluids. (American Society for Testing and Materials, Philadelphia, Pa. 19103).

  (a) D 240-64 Heat of Combustion of Liquid Hydrocarbon Fuels by Bomb Calorimeter;

  (b) D 2382-65 Heat of Combustion of Hydrocarbon Fuels by Bomb Calorimeter (High-Precision Method).

(3) R. S. Jessup, Precise Determination of Heat of Combustion by Bomb Calorimeter, Nat'l Bur. Standards Monograph 7, 1960. (U. S. Government Printing Office, Washington, D. C.).

21.6   Reaction Energy and Temperature

21.6.1   Effect of Temperature on Enthalpy of Reaction

The enthalpy change in a reaction (for instance, the enthalpy of combustion) is a function of the temperature at which the reaction occurs, and of the nature of the reacting substances. We may illustrate the relationships involved by reference to Figure 21.1. Figure 21.1 is a schematic diagram of enthalpy states of a system in which a reaction can occur and the temperature can change.

At T_1 the sum of the enthalpies of formation of the reactants may be represented as point A; the sum of the enthalpies of formation of the products by point B. The enthalpy change of the isothermal reaction, reactants → products, at T_1 is

$$\Delta H(B - A) = \Delta H(\text{reaction, at } T_1)$$
$$= \Sigma \Delta Hf(\text{products, at } T_1) - \Sigma \Delta Hf(\text{reactants, at } T_1) \qquad (1)$$
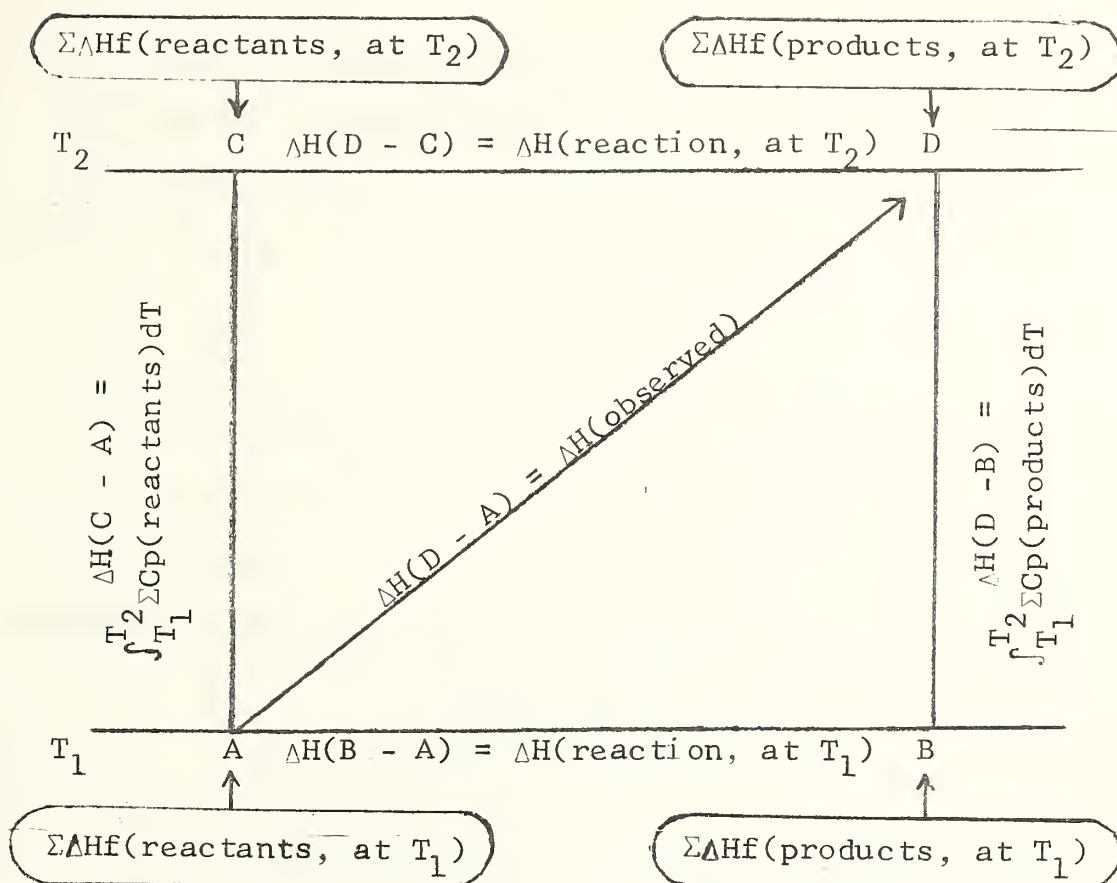
Figure 21.1 Effect of Temperature on Enthalpy of Reaction

A, B, C, D, are points on the state diagram for enthalpy
of a system in which a reaction can occur and the tem-
perature can change. An observed process, the transi-
tion from state A to state D can be resolved into two
components as shown. In one component the enthalpy
changes with composition, and in the other component the
enthalpy changes with temperature.

At T_2 the sum of the total enthalpies of formation of the reactants may be represented by point C; the sum of the enthalpies of formation of the products, by point D. The enthalpy change of the isothermal reaction, Reactants → Products, at T_2 is

$$\Delta H(D - C) = \Delta H(\text{reaction, at } T_2)$$

$$= \Sigma \Delta Hf(\text{products, at } T_2) - \Sigma \Delta Hf(\text{reactants, at } T_2) \qquad (2)$$

To heat the reactants from T_1 (point A) to T_2 (point C) requires that an enthalpy equal to the difference between C and A be added to the reactants. This enthalpy is mathematically given by the relationship:

$$\Delta H(C - A) = \int_{T_1}^{T_2} \Sigma Cp(\text{reactants}) dT \qquad (3)$$

or equally well
$$= \Sigma(H - H_0)(\text{reactants, at } T_2) - \qquad (3')$$
$$\Sigma(H - H_0)(\text{reactants, at } T_1)$$
$$= \Sigma(H - H_{298})(\text{reactants, at } T_2) - (3'')$$
$$\Sigma(H - H_{298})(\text{reactants, at } T_1)$$

Depending upon the availability of data, $\Delta H(C - A)$ may be evaluated by summing the enthalpy terms $H - H_0$ or $H - H_{298}$ or by summing and integrating the heat capacity terms. The term $\int_{T_1}^{T_2} \Sigma Cp(\text{reactants}) dT$ may be approximated over small temperature ranges by $\Sigma Cp(\text{reactants})(T_2 - T_1)$; that is, by assuming the Cp's are constant. (The abbreviation $\Sigma Cp(\text{reactants})$ should be understood to mean the total heat capacity of all the reactants, and so the individual heat capacities must be weighed according to the amounts of substance involved.)

To heat the products from T_1 (point B) to T_2 (point D) requires that an enthalpy equal to the difference between D and B be added to the products. This enthalpy is mathematically exactly given by the relationship:

$$\Delta H(D - B) = \int_{T_1}^{T_2} \Sigma Cp(products)dT \qquad (4)$$

or equally well
$$= \Sigma(H - H_0)(products, \text{ at } T_2) -$$
$$\Sigma(H - H_0)(products, \text{ at } T_1) \qquad (4')$$

or
$$= \Sigma(H - H_{298})(products, \text{ at } T_2) -$$
$$\Sigma(H - H_{298})(products, \text{ at } T_1) \qquad (4'')$$

The term $\int_{T_1}^{T_2}\Sigma Cp(products)dT$ may be approximated over small temperature ranges by $\Sigma Cp(products)(T_2 - T_1)$ that is, by assuming the Cp's are constant.

21.6.2 Relationships between Enthalpies of Isothermal Reactions at Different Temperatures

The difference in enthalpy between points D and A (Figure 21.1) is constant for a given reaction. Advantage may be taken of this fact to demonstrate a method of calculating the relationship between $\Delta H(reaction, \text{ at } T_1)$ and $\Delta H(reaction, \text{ at } T_2)$. The energy difference is independent of the path followed. Thus a path A → C → D may be followed or a path A → B → D may equally well be followed. An arbitrary path A → D, represented by the diagonal may also be followed. Mathematically:

$$\Delta H(D - A) = \Delta H(D - C) + \Delta H(C - A) \qquad (5)$$
$$= \Delta H(D - B) + \Delta H(B - A) \qquad (6)$$

Substituting quantities from the above discussion we have

$$\Delta H(D - A) = \Delta H(\text{reaction, at } T_2) + \int_{T_1}^{T_2} \Sigma Cp(\text{reactants})dT$$
$$= \int_{T_1}^{T_2} \Sigma Cp(\text{products})dT + \Delta H(\text{reaction, at } T_1) \qquad (7)$$

In the simple case where Cp's are independent of T_1 the above relationship is sometimes simplified to the following:

$$\Delta H(\text{reaction at } T_2) = \Delta H(\text{reaction at } T_1) + \Delta Cp(T_2 - T_1) \qquad (8)$$

in which ΔCp is the difference: heat capacity of products minus heat capacity of reactants.

21.6.3 Enthalpy Relations When the Temperature of the System is Allowed to Change (at Constant Pressure)

The enthalpy difference between point D and point A, $\Delta H(D - A)$ is a function only of the ingredients of the system and the temperatures T_2 and T_1. Pressure effects are negligible except in unusual cases. We shall consider only the isobaric process.[*] For a given system, the difference, $\Delta H(D - A)$, is dependent on T_2 and T_1. For a given system, if T_2 and T_1 are fixed, then $\Delta H(D - A)$ is also fixed. The relevant relationships are given by equation (7). If a reaction occurs in which the reactants are at T_1 (point A) and the products are at temperature T_2 (point D), the enthalpy change is $\Delta H(\text{observed})$.

This appears or is evident as heat, $Q = -\Delta H(\text{observed})$.

Two extreme cases can be recognized.

---

[*] The only work done is presumed to be pressure-volume work.

(a) <u>The adiabatic process.</u> No heat transfer between the system and the external world occurs in the adiabatic process. Mathematically this is equivalent to saying

$$Q = -\Delta H(observed) = 0$$

Since $\Delta H(observed) = \Delta H(reaction, at\ T_1) + \int_{T_1}^{T_2} \Sigma\ Cp(products)dT$ this means that for the adiabatic process, $-\Delta H(reaction, at\ T_1) = \int_{T_1}^{T_2} \Sigma\ Cp(products)dT$. This is a mathematical way of saying the enthalpy of reaction, being retained in the system, if exothermic causes the temperature of the products to rise an amount determined by their specific heat.

The temperature rise that will occur is often determined by a method of successive approximation. An estimate is made of the temperature rise. The specific heats are used to calculate the necessary $-\Delta H(reaction\ at\ T_1)$. If the value for $-\Delta H(reaction, at\ T_1)$ calculated in this way is less than the true value obtained from the Tables, the estimated temperature is increased, and the process repeated. If the value calculated for $-\Delta H(reaction, at\ T_1)$ is larger than the true value, the estimated temperature is decreased. The iteration is repeated until the calculated and tabular values of $-\Delta H(reaction, at\ T_1)$ are as close to one another as desired.

(b) <u>The isothermal process.</u> Heat transfer between the system and the external world is complete in the isothermal process, so that the temperature of the system always remains at T_1. No practical system is completely adiabatic, and more

or less heat transfer will be encountered in any real re-action process. At the other extreme, the amount of heat transferred equals the negative of the enthalpy of the isothermal process,

$$-Q = \Delta H(observed) = \Delta H(reaction\ at\ T_1) + \int_{T_1}^{T_2} \Sigma\ Cp\ (products)dT$$

Since $T_1 = T_2$ the second term of the right hand side is zero, and

$$Q = -\Delta H(reaction,\ at\ T_1)$$

The temperature rise of the products of reaction can be regulated by allowing the transfer of varying amounts of heat. The maximum possible temperature rise is, of course, the adiabatic temperature rise. This maximum temperature can be regulated to some extent by varying the composition of the system.

21.7 Reaction Equilibrium and Temperature

Data in the tables of this monograph and in additional tables of
thermal functions referred to in Section 22.0 are suitable for calculations
of thermodynamic equilibria at the final temperature in reactions involving
a few or many species. We limit ourselves here to a very brief outline
of the procedures and refer the reader to other sources for detailed
procedures. Several references to more detailed presentations of the
general problems of handling high temperature equilibria of multicomponent
systems are found in Section 24.0. Because several parameters must be
adjusted simultaneously or at least in a mutually consistent way and
because many variables are present in a multicomponent system, the solution
of such problems may be very time consuming and arduous unless assisted
by rapid machine calculation. The techniques for using such aids change
rather rapidly and the user may find being developed from time to time
procedures that are more efficient in the use of machine time. All dis-
cussion presented here is based on an assumption of equilibrium in the
gaseous state. Equilibrium may be quite closely reached in hot reacting
systems; but even in the absence of equilibrium the results of equilibrium
calculations may provide a useful approximation to the real situation.
There is currently much work being done on the application of thermodynamics
and kinetics to estimate dynamic non-equilibrium performance. Some such
work is described in references in Section 24.0 (see, for example,
references [5, 8, 29]).

When a complex mixture is allowed to react until it comes to equilib-
rium, two general limiting cases can be readily identified and
described. (1) The resulting temperature is determined by the energy

of reaction--no energy losses being allowed. (2) Energy exchange is
allowed, and the combustion products are brought to the same final tem-
perature as the initial temperature. These two situations represent the
adiabatic and isothermal process, respectively. The real situation lies
somewhere in between. There are always some heat losses to the surroundings.

The equilibrium thermodynamic state of the system comprising the pro-
ducts of combustion can be completely described by specifying the compo-
sition and enthalpies of the initial materials that have been burned and
the final pressure at which the products will be present. The final
temperature and product composition will then be given in terms of four
sets of simultaneous equations giving: (a) mass balance; (b) enthalpy
balance; (c) pressure balance; and (d) chemical equilibria.

(a) The equations for the conservation of mass are summarized as
equations (1A) and (1B).

$$\sigma_i = \sum_{k=1}^{\alpha} a_{ik} \, n_k \quad \text{for the reactants} \tag{1A}$$

As an initial step the number of gram-atoms, σ_i, of the i'th element, which
we shall identify as A_i, introduced into the reaction zone is calculated
from equation (1A); σ_i is the sum of the number of gram-atoms of A_i in
the substances introduced. There are α different substances introduced,
which we shall identify as B_k, and these are enumerated from k = 1 to k = α.
The number of moles B_k is n_k and the subscript of A_i in the chemical formula
of B_k is a_{ik}. If there are N elements present, i will range from 1 to N
and there will be N such equations.

As an example let us consider a combustion mix introduced into the
furnace and consisting of one kilogram of cellulose (monomer formula,

$C_6H_{10}O_5$; molecular weight, 242), one kilogram of benzene (formula, C_6H_6; molecular weight, 80), and thirty kilograms of combustion air (approximate formula, 78% N_2; 20% O_2; 2% H_2O; molecular weights, N_2, 28; O_2, 32; H_2O, 18).

The numbers of moles n_k of the various substances are calculated as follows [for simplicity approximate atomic weights are used]:

n_1 (cellulose) = 1000/242 = 4.13 moles

n_2 (benzene) = 1000/80 = 12.50 moles

n_3 (O_2) = (0.20) (30000/32) = 187.50 moles

n_4 (N_2) = (0.78) (30000/28) = 835.71 moles

n_5 (H_2O) = (0.02) (30000/18) = 33.33 moles

The numbers of gram atoms, σ_i, of the various elements are calculated as follows:

σ_1 (carbon) = 6(4.13) + 6(12.50) = 99.78 gram atoms

σ_2 (hydrogen) = 10(4.13) + 6(12.50) + 2(33.33) = 182.96 gram atoms

σ_3 (oxygen) = 5(4.13) + 2(187.50) + 33.33 = 428.98 gram atoms

σ_4 (nitrogen) = 2(835.71) = 1671.42 gram atoms

For this example N is 4 and α is 5.

Having established the composition of the combustion mix a necessary step in the calculation of the mass balance is to list the presumed reaction products to be considered. This is a critical step, depending upon the judgement of the individual; there being no way a priori to establish definitively what products will be formed.

Referring to the above example we shall expect to find CO_2, H_2O, O_2, and N_2 as major components of the combustion products. However, if care is to be used in controlling effluent gases we must also take into account

the possibility of formation of CO, NO, NO_2, and HNO_3. As a matter of pro-
cedure we shall also consider the gaseous monatomic elements, C,O,N,H,
as being present. If the amount of oxygen is limited, one must also
consider such possibilities as unburned or partially burned ingredients
such as gaseous H_2, CH_4, CH, C_2, C_2H_2, and HCO. There are a very large
number of potential components resulting from incomplete combustion.
The variety of potential products of combustion will increase rapidly as
additional elements are included in the combustion mixture.

When this has been done, the number of gram-atoms of the elements
can be expressed as the sum of their presence in the products of combustion
by equation (1B).

$$\sigma_i = \sum_{j=1}^{\beta} a_{ij}\, n_j \quad \text{for the combustion products} \tag{1B}$$

In equation (1B), σ_i is the same series of quantities calculated by
equation (1A). There are β presumed products of combustion, and there
are n_j moles of product B_j in the formula in which the subscript of the
element A_i is a_{ij}.

Equations (1B) become:

$$\sigma_1 \text{ (carbon)} \quad = n_C + n_{CO} = n_{CO_2} + n_{CH_4} + n_{CH} + 2n_{C_2} + 2n_{C_2H_2} + n_{HCO}$$

$$\sigma_2 \text{ (hydrogen)} = n_H + 2n_{H_2} + 2n_{H_2O} + 4n_{CH_4} + n_{CH} + 2n_{C_2H_2} + n_{HCO} + n_{HNO_3}$$

$$\sigma_3 \text{ (oxygen)} \quad = n_O + 2n_{O_2} + n_{NO} + 2n_{NO_2} + n_{H_2O} + 3n_{HNO_3} + n_{CO} + 2n_{CO_2} + n_{HCO}$$

$$\sigma_4 \text{ (nitrogen)} = n_N + 2n_{N_2} + n_{NO} + n_{NO_2} + n_{HNO_3}$$

The values assigned to the n's cannot be made final without solving the
equilibrium equations.

(b) Equation (2) is the equation for the conservation of energy in the case where all energy of reaction goes to heating the products of combustion.

$$\sum_{k=1}^{\alpha} n_k \left[\Delta Hf^{\circ}_{298} \text{ of } B_k + (H_{T_1} - H_{298}) \text{ of } B_k \right]$$
$$= \sum_{j=1}^{\beta} n_j \left[\Delta Hf^{\circ}_{298} \text{ of } B_j + (H_{T_2} - H_{298}) \text{ of } B_j \right] \qquad (2)$$

As before there are α ingredient substances (or reactants) B_k in the combustion mix, and these are enumerated from $k = 1$ to $k = \alpha$. The enthalpy contribution of each ingredient is given by a term on the left hand side of the equation and consists of the number of moles n_k times its enthalpy of formation at 298 K plus an enthalpy increment if the initial temperature T_1 of the ingredients differs from 298 K.

The enthalpy requirements to form the products of combustion and bring them to the final temperature T_2 are given by the right hand side of the equation. There are β combustion products B_j and these are enumerated from $j = 1$ to $j = \beta$. The enthalpy requirement for each combustion product is given by a term which consists of the number of moles n_j times its enthalpy of formation at 298 K plus an enthalpy increment to bring its final temperature to T_2.

Note that the number of moles of each substance formed in the products will depend upon the temperature of the products, and this dependence will be particularly pronounced if some comparatively unstable combustion products can be formed. Therefore the quantities n_j must be made consistent with the requirements of the possible equilibria at the final temperature. The quantities n_k, on the other hand, depend only on the mixture burned.

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Note also that if energy losses occur, such as losses through the furnace walls, the final temperature T_2 will not be as high as if there were no such losses.

(c) Equation (3) is the pressure balance equation.

$$P_t = \sum_{j=1}^{\beta} P_j \tag{3}$$

In equation (3) P_t is the total pressure in the chamber where the combustion products are present, and P_j is the partial pressure of the j'th product, B_j. The partial pressures are given in terms of the number of moles and the total pressure by equation (3'), assuming the fugacities

$$\frac{P_j}{P_t} = \frac{n_j}{\sum_{j=1}^{\beta} n_j} \tag{3'}$$

are all proportional to the pressures. Note that the partial pressures can be calculated only after the mole ratios are known.

(d) Equations (4) and (4') are the equations for the reaction equilibria involved. There are various ways in which the equilibria may be specified. An unambiguous way which assures that all possible equilibria are implicitly included is to give the equilibrium constant of formation of each substance from the atoms of the elements present.

$$RT \ln K_j = RT \ln f_j - \sum_{i=1}^{N} a_{ij} \ln f_i \tag{4}$$

$$RT \ln K_j = (-\Delta Hf^\circ_o)_j - (G^\circ_T - H^\circ_o)_j + \sum_{i=1}^{N} a_{ij} [(\Delta Hf^\circ_o)_i + (G^\circ_T - H^\circ_o)_i] \tag{4'}$$

The constant K_j is the equilibrium constant of formation of B_j, the j'th constituent of the products, from the atoms of the elements. There are

N elements present, and so for each substance present the elements in it
are enumerated from i = 1 to i = N. The coefficient a_{ij} represents the
subscript of element i in the formula for the substance B_j. The equilibrium
constant can be expressed in two ways represented by equations (4) and (4')
respectively. Equation (4) represents the definition of the equilibrium
constant of formation from the gaseous monatomic elements in terms of the
fugacities of the elements and of the combustion products, f_i and f_j,
respectively. Equation (4') represents the equilibrium constant in terms
of the Gibbs energies of the substance and of the elements respectively,
and the enthalpy of reaction, which can be derived from the enthalpies of
formation of the substance and the elements respectively. The reader
should note that the elements as used in the equations (4) and (4') are not
in their standard reference states, but are in the form of the gaseous
monatomic species. The elimination of RT ln K_j from equations (4) and (4')
allows a single equation to represent the equilibrium for each reaction.
For gases at not too high pressures the fugacity equals the pressure
(i.e., $f_j = P_j$). For gases to which this equality does not apply, a
correction term may have to be applied. For condensed phase products
formed f_j is considered to be unity.

We may illustrate the equilibria involved in the previous example
in the following way:

$$2H(g) \rightleftarrows H_2(g)$$
$$2O(g) \rightleftarrows O_2(g)$$
$$2N(g) \rightleftarrows N_2(g)$$
$$2H(g) + O(g) \rightleftarrows H_2O(g)$$

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$$C(g) + O(g) \rightleftharpoons CO(g)$$

$$C(g) + 2O(g) \rightleftharpoons CO_2(g)$$

$$N(g) + O(g) \rightleftharpoons NO(g)$$

$$N(g) + 2O(g) \rightleftharpoons NO_2$$

$$C(g) + 4H(g) \rightleftharpoons CH_4(g)$$

$$C(g) + H(g) \rightleftharpoons CH(g)$$

$$2C(g) \rightleftharpoons C_2(g)$$

$$2C(g) + 2H(g) \rightleftharpoons C_2H_2(g)$$

$$H(g) + C(g) + O(g) \rightleftharpoons HCO(g)$$

$$H(g) + N(g) + 3O(g) \rightleftharpoons HNO_3(g)$$
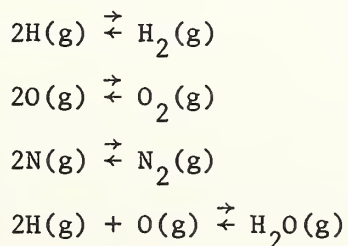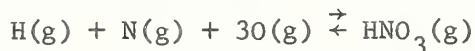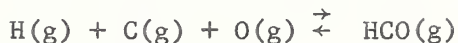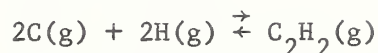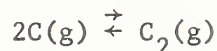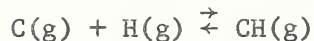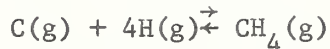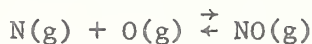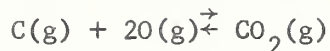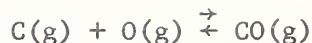
This sequence of reaction is sufficient to specify the equilibria involving the formation of the substances specifically listed above. It will be apparent from the above sequence of reactions that a number of the proposed species will be found only in extremely small quantities and a way can probably be found to reduce the number of equations by eliminating these species. In addition, it can easily become apparent that one or more additional species are important enough for inclusion. The criteria for inclusion will differ for different species depending upon contribution to the mass or pressure balance, toxicity, corrosiveness or other factors. The equilibria shown were chosen as a systematic way of identifying unambiguously a sufficient number of non-redundant equations including all the substances under consideration. An attempt to write down directly the equilibria that are of real importance may lead to problems because of redundancies or because they form an insufficient set. Provided that all substances of importance have been listed a set involving formation of a substance from the gaseous atoms such as those given above, includes implicitly or explicitly all equilibria of importance.

The mass balance equations for the combustion products can now be listed.

$$\sigma_1 \text{ (carbon)} = n(C) + n(CO) + n(CO_2) + n(CH_4) + n(CH) + 2n(C_2)$$
$$+ 2n(C_2H_2) + n(HCO)$$

$$\sigma_2 \text{ (hydrogen)} = n(H) + 2n(H_2) + 2n(H_2O) + n(HNO_3) + 4n(CH_4) + n(CH)$$
$$+ 2n(C_2H_2) + n(HCO)$$

$$\sigma_3 \text{ (oxygen)} = n(O) + 2n(O_2) + n(H_2O) + n(CO) + 2n(CO_2) + n(NO)$$
$$+ 2n(NO_2) + n(HCO)$$

$$\sigma_4 \text{ (nitrogen)} = n(N) + 2n(N_2) + n(NO) + n(NO_2) = n(HNO_3)$$

The pressure balance equation can be written:

$$P_t = P(C) + P(CO) + P(CO_2) + P(CH_4) + P(CH) + P(C_2) + P(C_2H_2)$$
$$+ P(HCO) + P(H) + P(H_2) + P(H_2O) + P(O) + P(O_2) + P(NO)$$
$$+ P(NO_2) + P(HNO_3) + P(N) + P(N_2).$$

An iterative procedure for calculating equilibrium compositions and energies is as follows:

(1) Prepare equations for reactions that may participate in equilibria at the resulting temperature.

(2) Write mass balance equations for each element in terms of molecular species present based on combustion ingredients introduced.

(3) Write expressions for equilibrium constants.

(4) Assume a temperature T_2 and a number of moles for each product and try the consistency of the equations. Calculate the number of moles of gas and test the material balance. If material imbalances result adjust n. When n has been adjusted to balance, the temperature, T_2 and

moles of products n_j are consistent. This gives a product profile for a given T_2. However, T_2 may be incorrect for the enthalpy. Calculate the enthalpies of the products at T_2 (including enthalpies of formation and enthalpy increments to T_2).

(5) Then repeat determinations of product profiles until enthalpies of products and of reactants are equal. This gives the correct T_2, and the remaining quantities, moles of each product, partial pressures, etc., are then correct.

A different approach is to find the composition of the combustion which minimizes Gibbs energy of the system. This approach is discussed in References [33] and [34] of Section 24.0. Only the principle of this method will be mentioned here. The procedures for carrying out a calculation may be found in reference [33].

The condition for a minimum (or a maximum) in a mathematical function is that the derivative or differential be zero. The condition for thermochemical equilibrium is that the Gibbs energy, dG, be a minimum for the system. This is expressed by the statement which sets the differential equal to zero (equation (5))

$$dG = 0 \tag{5}$$

At a fixed temperature and pressure and for a specified set of combustion products B_j the differential dG is given by equation (6).

$$dG = \sum_{j=1}^{\beta} \mu_j \, dn_j \tag{6}$$

Here dn_j is a differential change in the number of moles n_j of component B_j, and μ_j is the chemical potential of the species B_j. The chemical

potential of B_j is the differential rate of change of the Gibbs energy of the system per mole of B_j added to the system (equation (7)).

$$\mu_j = \frac{\partial G}{\partial n_j} \qquad (7)$$

For an ideal gas :

$$\mu_j = G_j^\circ + RT \ln P_j$$

This system is subject to the same constraints as before, that the mass balance must be maintained and that the energy balance must be maintained.

By consideration of all of the possible chemical products and maintaining the mass balance of the elements present, a set of mole numbers for the combustion products can be calculated which leads to a minimum Gibbs energy and equilibrium temperatures for the whole system by an iterative process.

22.0   Supplementary Sources of Thermodynamic Data
on Chemical Substances and Materials

The following monographs are collections of thermodynamic data compiled from the original literature by competent thermochemists and presented in a well organized way. These sources have been selected to provide reasonably comprehensive coverage but are by no means a complete list of compilations of thermodynamic data. Except for the Landolt-Börnstein tables, foreign language compilations have not been included because of their limited accessibility. The extensive Russian compilations of thermodynamic tables are essentially very similar to some of the more comprehensive compilations listed here. Two general texts on thermodynamics and thermochemistry are also included.

1.   Ashcroft, S. J., and Mortimer, C. T.

Thermochemistry of Transition Metal Complexes

(Academic Press, London, New York, 1970).

This book surveys the literature to 1968 on energy processes involving transition metal complexes including both organic and inorganic ligands. A critical review of the thermochemical data for over 1500 systems of complexes is given. Comparable data from various sources are shown in juxtaposition. Values of ΔH, ΔG, and ΔS for various stages of complex formation are usually listed for processes in aqueous solution. $\Delta Hf°$, $\Delta Gf°$, $\Delta Sf°$ for crystalline complex substances are given where available. In many instances correlations of the data for various metals with a single ligand, and for various related complexes of a given metal, are given graphically or by means of bond-energy estimates based on the data.

2. Bain, R. W.

    National Engineering Laboratory (NEL) Steam Tables, 1964

    Physical Properties of Water and Steam 0-800°C, 0-1000 Bars

    (Her Majesty's Stationary Office, Edinburgh)

These are typical steam tables, with data tabulated in SI units, except that pressure is in bars and temperature in °C. The tables were ratified by the Sixth International Conference on the Properties of Steam. An introduction to the tables is given. See also sources (8, 13).

3. Cox, J. D., and Pilcher, G.

    Thermochemistry of Organic and Organometallic Compounds

    (Academic Press, London, New York, 1970)

This monograph is a critcal compilation of thermochemical data published since 1930. The heats of formation of some 3000 substances are listed, with estimates of error. Where enthalpies of vaporization are known or can be reliably estimated these are listed and in these cases the enthalpies of formation of both gaseous and condensed phases are given. Extensive introductory material presents experimental procedures and procedures for reduction of experimental data of the type found in the book. Applications of thermochemical data are given, and there is a section on methods of estimating enthalpies of formation of organic compounds.

4. Domalski, E. S.

    Selected Values of Heats of Combustion and Heats of Formation

    of Organic Compounds Containing the Elements C, H, N, O, P, and S.

    (Journal of Physical and Chemical Reference Data $\underline{1}$, 221-277 (1972))

    Selected values of the enthalpies of combustion and enthalpies of
formation of 719 organic compounds are reported. These are essentially
the same as in the present compilation, but the selected values are
augmented by commentary and original source references. The Wiswesser
Line Notation is also given for each compound. The methods used in
updating older work are described.

5. Hilsenrath, J., Beckett, C. W., Benedict, W. S., Fano, L.,

    Hoge, H. S., Masi, J. F., Nuttall, R. L., Touloukian, Y. S.,

    and Woolley, H. W.

    Tables of Thermal Properties of Gases

    National Bureau of Standards Circular 564, (1955)

    (U. S. Government Printing Office, Washington, D. C. 20402)

    This monograph gives tables of compressibility factor, density,
entropy, enthalpy, specific heat, specific-heat ratio, and sound velocity
for the real gases: air, argon, CO_2, CO, H_2, N_2, O_2, and steam over
the range 0.01 to 100 atm and to 3000 K (in most cases). It also gives
ideal-gas thermodynamic functions to 5000 K. Vapor pressures, thermal
conductivity, viscosity and Prandtl number are given over the range of
available experimental data. Critical commentaries and descriptions
of the analyses of the data are provided.

6. Hultgren, R., Orr, R. L., Anderson, P. D., and Kelley, K. K.

    Selected Values of Thermodynamic Properties of Metals and Alloys

    (John Wiley and Sons, Inc., New York, London, 1963).

This volume gives the results of critical evaluations of the thermo-dynamic properties of the 63 metallic elements and 168 alloy systems. Self-consistency of the data, consistency with known thermodynamic relationships, consistency with known phase diagrams, and agreement between similar measurements, formed the bases for selection of the values. Heat capacities (Cp) at low and high temperatures and vapor pressure data are reviewed and references are given. Values are tabu-lated for Cp, $H_T - H_{298}$, and $-(G_T - H_{298})/T$, for condensed and gas phases, with T as the principal variable; and values of P, ΔG, and ΔH of the vaporization process are given. Values for $H_{298} - H_0$, S_{298}, T_m, ΔH_m and ΔS_m, and analytical expressions for $H_T - H_{298}$ as functions of T are given.

A supplement containing information on three additional elements and 4 alloy systems was issued in 1966.

7. Joshi, R. M., and Zwolinski, B. J.

    Vinyl Polymerization, Volume 1, Part I, edited by G. E. Ham

    (Marcel Dekker, Inc., New York, 1967)

    Chapter 8: Heats of Polymerization and their Structural and

    Mechanistic Implications

The authors discuss experimental methods used to measure and derive heats of polymerization. A listing of experimental data on heats of

polymerization is provided for 81 organic polymerization reactions.
Other tables give heats of formation, heats of vaporization, entropies,
Gibbs' energies, equilibrium constants, rate constants and activation
energies at 25°C for a variety of polymerization processes. A discussion
of the structural influence upon the heat of polymerization is also given.
At the end of the chapter, 164 references are cited.

8(a). Keenan, H. J., Keyes, F. G., Hill, P. G., and Moore, J. G.

Steam Tables

Thermodynamic Properties of Water, including Vapor, Liquid, and

Solid Phases (International Edition, Metric Units)

(John Wiley and Sons, Inc., New York, London, Sydney, Toronto, 1969)

This book presents the results of a new and independent correlation
of all the new thermodynamic data and all previously existing data. It
constitutes a complete revision of the Keenan and Keyes Tables of 1936 and
an extension of range to 1000 bars and about 1300°C.

Values of the thermodynamic properties specific volume, internal
energy, enthalpy, and entropy are tabulated with pressure and temperature
as parameters, for vapor-liquid equilibrium, vapor-solid equilibrium,
superheated vapors, and compressed liquid. Mollier and temperature-entropy
charts are included along with charts of heat capacity of liquid and vapor,
Prandtl number, and isentropic expansion coefficient. A detailed table
for the critical region shows volume and temperatures as parameters.

The present tables are in no sense a formulation of the International
Skeleton Tables (1963). In general they are in good accord with, and their
values fall within the tolerance of the International Skeleton Tables.

Exceptions are discussed. Extensive tables of viscosity and thermal
conductivity are reproduced from the documents of the Sixth International
Conference on the Properties of Steam.

Energy units are joules, temperatures are K or °C, pressures are in
bars, volumes in cm^3 and masses in grams. The data and tables are dis-
cussed in an appendix of 25 pages; and a list of 37 references is given.
The introduction is in English, French, German, Italian, Japanese, Russian,
and Spanish. See also sources (2, 13).

8(b). Keenan, J. H., Keyes, F. G., Hill, P.G., and Moore, J. G.

  Steam Tables

  Thermodynamic Properties of Water, including Vapor, Liquid,

    and Solid Phases (English Units)

  (John Wiley and Sons, Inc., New York, London, Sydney, Toronto,

    1969).

This edition of the Steam Tables supplies the same basic information
as source (8a) except that English units are used.

A review of the sources of data and comparison of derived tabulated
values with experiment, and a summary of the equations used in deriving
the tabulated data are given in an appendix of 29 pages. Tables for the
vapor give specific volume, specific internal energy, specific enthalpy,
and specific entropy at temperatures from 32° to 2400°F, and at pressure
intervals from 0.2 to 15,000 lb/in^2; as well as several properties of the
very low pressure gas. Similar tables are given for the liquid, covering
somewhat different ranges. See also sources (2, 13).

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9. Kelley, K. K.

    Contributions to the Data on Theoretical Metallurgy

    XV. A Reprint of Bulletins 383, 384, 393, and 406

    Bureau of Mines Bulletin 601 (1962)

    (U. S. Government Printing Office, Washington, D. C.)

    This monograph is a reprint collection of previous monographs having
the same principal title. The subtitles of these are listed below.

    III. The Free Energies of Vaporization and Vapor Pressures of

        Inorgnic Substances. Bureau of Mines Bulletin 383 (1935).

    IV. Metal Carbonates--Correlations and Applications of Thermodynamic

        Properties. Bureau of Mines Bulletin 384 (1935).

    V. Heats of Fusion of Inorganic Substances. Bureau of Mines

        Bulletin 393 (1936).

    VII. The Thermodynamic Properties of Sulfur and Its Inorganic

        Compounds. Bureau of Mines Bulletin 406 (1937).

This volume together with Bureau of Mines Bulletins 542, 584, and 592
constitute a complete set of the thermodynamic data series.

A typical presentation of the selected data for vaporization gives
$C_p(g)$, $C_p(liq)$, $C_p(c)$, ΔC_p, ΔH_{vap}, ΔG_{vap} as analytical equations in
temperature, and values of ΔH_{298}, S_{298}, and T_b. The monograph on metal
carbonates gives selected values and equations for C_p, S, ΔG_f°, ΔH_f°
for CO, CO_2, H_2O, carbonate(aq) and bicarbonate(aq) ions, and 25 metal
carbonates or bicarbonates. A table of dissociation pressures is given.
The monograph on enthalpies of fusion gives selected values of ΔH_m for

63 elements and many of their compounds. The monograph on sulfur compounds gives similar information for elemental sulfur, a few gaseous non-metallic compounds, and for the sulfides and sulfates. Illustrations of the uses of thermochemical data, critical discussions of the source data, and bibliographies are given in each monograph.

10. Kelley, K. K.

   Contributions to the Data on Theoretical Mettalurgy

   XIII. High-Temperature Heat-Content, Heat-Capacity, and Entropy

     Data for the Elements and Inorganic Compounds.

   Bureau of Mines Bulletin 584, (1960).

   (U. S. Government Printing Office, Washington, D. C.)

This comprehensive monograph gives procedures used in the correlations, and gives selected values, tables, and analytical functions in temperature for the subject thermodynamic data of several hundred substances. A bibliography of sources is provided. The breadth of coverage is very great. Substances for which data are provided include the first 92 elements and many of their acids, oxides, carbides, nitrides, hydrides, hydroxides, halides, carbonates, nitrates, phosphates, sulfates, borates, cyanides, mixed oxides and intermetallic compounds.

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11. Kubaschewski, O., Evans, E. Ll., and Alcock, C. B.

     Metallurgical Thermochemistry, 4th Edition

     (Pergamon Press, Oxford, New York, and other cities, 1967)

This monograph is a standard reference work for metallurgists, and deals with the thermochemistry in a rather broad way with special emphasis on inorganic compounds and alloys. About 140 pages of tables of thermochemical data are given in which are presented ΔHf°_{298}, S°_{298}, T_{trans}, T_m, T_b, structural information, ΔH_m, ΔH_{vap}, and ΔH_{subl}, for elements and compounds.

Constants of analytical expressions for Cp, the vapor pressure, and ΔGf° or ΔG for a reaction, with temperature as the variable, together with the temperature range of applicability, are given for many substances. A separate table gives the thermodynamic properties of mixing for alloys. The tabulated data are derived from other compilations and the original literature.

The accompanying text, comprising some 300 pages, gives the theoretical basis of the deviation and application of thermochemical data, a discussion of the estimation of thermochemical data, and examples of thermochemical treatment of metallurgical problems.

12. Merrill, A. L., and Watt, B. K.

     (a) Energy Value of Foods; Basis and Derivation
          Agriculture Handbook No. 74, 1955.

     (b) Watt, B. K., and Merrill, A. L.
          Composition of Foods; Raw, Processed, Prepared
          Agriculture Handbook No. 8, revised, 1963

          (U. S. Government Printing Office, Washington, D. C. 20402)

This pair of monographs provides numerous composition and energy values for food and foodstuff ingredients. It should be noted, of course, that the Calorie used in food energy values is 1 kcal as used in this handbook. In Agriculture Handbook No. 74, Part I gives a discussion of the sources of food energy in terms of organic compound class, and of the experimental determination of heats of combustion. Parts II, III, and IV apply the data to physiological processes. An appendix gives composition and heat of combustion of foods. Tables 1-5 and table 24 give heats of combustion of specific food items or component substances. Care should be used in taking values from the numerous tables, as correction factors have sometimes been applied to adjust for physiological processes. These adjustments are indicated by footnotes. In Agriculture Handbook No. 8, Appendix A is of particular interest as it gives notes on energy values and nutrients, including (adjusted) heats of combustion of many foods and food ingredients.

13. Meyer, C. S., McClintock, R. B., Silvestri, G. J., and Spencer, R. C., Jr.

    ASME Steam Tables 1967

    Thermodynamic and Transport Properties of Steam; comprising Tables and Charts for Steam and Water

    (American Society of Mechanical Engineers, New York, N.Y., 10017)

These tables give an introductory discussion of their source. Nine tables and thirteen charts of thermodynamic properties are given. The data were computed from equations adopted in the IFC*, Formulation for

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*International Formulation Committee of the Sixth International Conference on the Properties of Steam.

Industrial Use, which is reproduced. Reference is made to computer procedures for handling the source equations. Three tables of transport properties are given, based on the skeleton tables and empirical equations developed by the Sixth International Conference. The principal tables are in U. S. Customary units. See also sources (2, 8).

14. Pitzer, K. S., and Brewer, L.

Thermodynamics: Gilbert N. Lewis and Merle Randall (Second edition) (McGraw Hill Book Company, Inc., New York, Toronto, London, 1961)

This monograph on thermodynamics and its application to physics and chemistry is a revision and updating of the classical work by Lewis and Randall, that did much to shape the development of thermodynamics in the 20th century. It provides a reasonably complete presentation of the principal subjects of thermodynamics. In addition it provides in the appendices (among other subjects) tables and discussions of (1) properties of normal solutions, (2) properties of gaseous solutions, (3) a tabular summary of thermodynamic formulas, (4) tables of thermodynamic properties. The latter tables include ΔHf°_{298} and $-(G^{\circ} - H^{\circ}_{298})/T$ for halides, oxides, sulfides and related compounds, carbides, and nitrides, at 298, 500, 1000, 1500, and 2000 K. Values of $-(G - H^{\circ}_{0})/T$ at the same temperatures, $H^{\circ}_{298} - H^{\circ}_{0}$, and ΔHf°_{0} are given for some of the elements. Also, $-(G - H^{\circ}_{0})/T$ at the same temperatures, ΔHf°_{298}, ΔHf°_{0}, and $H^{\circ}_{298} - H^{\circ}_{0}$ are given for some gaseous carbon compounds, halides, oxides, hydrides, and related compounds. Sources of data are given.

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careful studies, many of which were done in connection with the same API

Research Project. Experimental data are supplemented by theoretical

calculations or empirical correlations. References to the source data

and a bibliography are given. The data in many instances are identical

to those in NBS Circular C461, listed above. See also source (15).

17. Rossini, F. D., Wagman, D. D., Evans, W. H., Levine, S., and Jaffe, I.

Selected Values of Chemical Thermodynamic Properties   .

National Bureau of Standards Circular 500 (1952)

(U. S. Government Printing Office, Washington, D. C. 20402)

This was for many years the most comprehensive authoritative compila-

tion of thermochemical data at 298.15 K for inorganic substances. All

inorganic substances and organic substances containing two carbon atoms

or fewer per molecule are included if thermodynamic data exist for calcu-

lating one of the properties tabulated. Properties tabulated in Part I

are ΔHf°_{0}, ΔHf°_{298}, ΔGf°_{298}, log Kf, S°_{298}, and Cp°_{298}. Properties tabulated

in Part II are temperature, pressure, enthalpy change, entropy change

and heat capacity change for the phase changes: transition, fusion, and

vaporization. The data from original sources were critically evaluated

by competent thermochemists and best values selected for the functions

tabulated, maintaining internal consistency by the relationship: ΔGf°_{298} =

$\Delta Hf^{\circ}_{298} - T \Delta S^{\circ}_{298}$. The sources of data for each data item are listed and

a bibliography is included. Some information in this book can still

not be found readily elsewhere as the revision is not yet complete.

See Wagman, et al, (source [24]) below.

18. Schäfer, D., and Lax, E. (editors)

Landolt-Börnstein

Zahlenwerte und Fuçtionen aus Physik, Chemie, Astronomie,

Geophysik, und Technik, Sechste Auflage

Eigenschaften der Materie in Ihren Aggregatzuständen

4 Teil, Kalorische Zustandgrössen

(Springer-Verlag, Berlin, Göttingen, Heidelberg, 1961)

This most recent issue of thermodynamic information of the famous
Landolt-Börnstein series gives thermal properties: molar heat capacity,
entropy, enthalpy, enthalpy of formation, Gibbs energy of formation,
in the standard state, and enthalpies of phase changes for many organic
and inorganic substances in SI units. The dependence of thermal func-
tions and heat capacity upon temperature is given for many substances.
Some other thermodynamic quantities are given. Extensive tables are
given of group contributions to enthalpy of formation and the Gibbs
energy of formation of organic substances (gases) in $kcal\ mol^{-1}$ and
$kJ\ mol^{-1}$. Many of the heat capacity data are presented in diagrams.

19. Stern, K. H., and Weise, E. L.

High Temperature Properties and Decomposition of Inorganic Salts

Part 1. Sulfates - NSRDS-NBS-7 (1966)

Part 2. Carbonates - NSRDS-NBS-30 (1969)

(U. S. Government Printing Office, Washington, D. C.)

These two monographs treat the thermodynamics and kinetics of decomposition of sulfates of over 60 metals, and carbonates of over 21 metals in a systematic way. The general features of the decomposition chemistry, phase transition temperatures, densities, and decomposition equilibria as functions of temperature are discussed. Also the mechanism of endothermic solid state decomposition, kinetic equations, and surface area changes during decomposition, and several parameters affecting rate of decomposition are discussed. These parameters include pressure, activation energy, method of preparation, heat transfer and crystal imperfections. Data given for each of the substances involved include density, thermal expansion coefficient, transition temperatures, entropy at 298 K, enthalpy of formation at 298 K, as well as the following functions of temperature: Gibbs energy of decomposition, equilibrium constant K and Log K of decomposition, and the Gibbs energy functions $-(G^{\circ} - H^{\circ}_{298})/T$. The coverage is not uniform as all the data have not been measured for all the compounds. The substances involved are SO_3, SO_2, O_2, CO_2, CO, the carbonates, the sulfates, and the oxides. The values obtained are the results of a critical review of the original literature sources.

20. Stull, D. R., and Prophet, H., editors

     JANAF Thermochemical Tables, 2nd Edition, 1971

     National Standard Reference Data Series NSRDS-NBS 37, (1971)

     (U. S. Government Printing Office, Washington, D. C. 20402)

This work appeared first as a series of loose-leaf data sheets, revised at intervals as new information became available. Each sheet

was dated. The first bound edition of the work (1965–1966) was issued
by the Clearinghouse for Federal Scientific and Technical Information
(since changed to: National Technical Information Service) as Document
PB-168370 and supplements. This has been somewhat revised for the second
edition. Approximately 1000 compounds, elemental molecules, and atomic
species, including a few gaseous ions, are included in this work. The
elements included were selected for relevance in rocket propellant
ingredients or products of combustion, and hence the elements of lower
atomic weight and substances formed from them predominate. However a
few heavier elements such as Pb, Hg, and W are included. Thermal functions
$Cp°$, $S°$, $-(G° - H°_{298})/T$, $H°-H°_{298}$, $\Delta Hf°$, $\Delta Gf°$, and Log Kp are tabulated
from 0 to 6000 K or to a lower temperature limit of meaningful data.
$\Delta Hf°$ at 0 K and 298 K, $S°_{298}$, ΔH_m and T_m as well as spectroscopic informa-
tion needed for statistical mechanical computation of thermodynamic
properties are listed. The sources of data are listed and briefly
discussed. A lengthy introduction discusses sources, methods of treatment,
and methods of application of the tables.

21. Stull, D. R., and Sinke, G. H.

    Thermodynamic Properties of the Elements

    Advances in Chemistry Series, Number 18

    (American Chemical Society, Washington, D. C., 1956)

    Tabulated values of $Cp°$, $H° - H°_{298}$, $S°$, $-(G° - H°_{298})/T$, $\Delta Hf°$, $\Delta Gf°$,
and log Kf are given for the solid, liquid, and gas states of the first
92 elements over the temperature range 298 to 3000 K. Also given, where

available, are $H_{298}^{\circ} - H_{0}^{\circ}$, temperatures of phase changes and the associated enthalpy changes, and critical constants. The source data for each element are cited and briefly discussed. While now 15 years old, this book is still the most convenient reference for high temperature properties of some of the heavier elements.

22. Stull, D. R., Westrum, E. F., and Sinke, G. H.

    The Chemical Thermodynamics of Organic Compounds

    (John Wiley and Sons, Inc., New York, London, Sydney, Toronto, 1969)

This monograph is divided into three parts. The first part gives theoretical basis and principles of thermodynamics and thermochemistry, some experimental and computational methods used, and some applications to industrial problems. The second part gives thermal and thermochemical properties in the ideal gas state from 298 to 1000 K. In this section, the sources of data are listed and discussed and standardized tables are presented for 918 organic compounds. Values of C_p°, S°, $-(G - H_{298}^{\circ})/T$, $H^{\circ} - H_{298}^{\circ}$, ΔH_f°, ΔH_f°, ΔG_f°, and log Kp are given at 100 K intervals. In the third section are listed selected values of enthalpy of formation, entropy, and consistent values of ΔG_f° and log Kp of organic compounds at 298 K. In excess of 4000 compounds are listed. A very few inorganic compounds are also found in this book. A chapter very briefly discusses methods of estimating thermodynamic quantities.

23. Touloukian, Y. S.

Retrieval Guide to Thermophysical Properties Research Literature

(McGraw Hill Book Co., New York, 1960-   )

These volumes, which are a continuing series, contain thoroughly cross-indexed references to the source literature for bulk transport and thermodynamic properties. The properties first covered are: thermal conductivity, specific heat, viscosity, thermal radiative properties, thermal diffusivity, diffusivity, diffusion coefficient, and Prandtl number. A limited but continually increasing number of data sheets are available on materials and pure substances, giving charts and tabulated values based on a critical evaluation, analysis, and correlation of existing data. These are separately supplied by the Thermophysical Properties Research Center (Purdue University) on a subscription basis. These comprise the Data Book: Volume I, Metallic Elements and Their Alloys; Vol. II, Non-metallic Elements, Compounds, and Mixtures (in Liquid and Gaseous States at Normal Temperature and Pressure); and Vol. III. Non-metallic Elements, Compounds, and Mixtures (in the Solid State at Normal Temperature and Pressure).

24. Wagman, D. D., Evans, W. H., Parker, V. B., and (in various individual parts) Halow, I., Bailey, S. M., Schumm, R. H., Churney, K. L.

Selected Values of Chemical Thermodynamic Properties

National Bureau of Standards Technical Note 270, October 1965

(and continuing)

(U. S. Government Printing Office, Washington, D. C. 20402)

This technical note is a revision of NBS Circular 500 Part I (see above) and is issued in parts as segments of the work relating to selected sequences of elements are completed. The following parts had been issued as of 1971.

270-1   Tables for the first twnety-three elements in the standard order of arrangement

270-2   Tables for elements 24-32 -- elements in the standard order of arrangement

270-3   Tables for the first thirty-four elements in the standard order of arrangement

270-4   Tables for elements 35-53 in the standard order of arrangement

270-5   Tables for elements 54-61 in the standard order of arrangement

270-6   Tables for the alkaline earth elements, elements 92-97 in the standard order of arrangement.

The remaining elements will be covered in two or three additional parts to appear over a period of about two years. Documentation and references have not yet been issued.

This is the most comprehensive recent compilation in English of critically evaluated thermochemical data at 298.15 K for inorganic substances. All inorganic substances and organic substances containing two carbon atoms or fewer per molecule are include if thermodynamic data exist for calculating any of the properties tabulated. The coverage when complete will be approximately 12,000 substances. Properties tabulated are ΔHf°_{0}, ΔHf°_{298}, ΔGf°_{298}, $H^{\circ}_{298.15} - H^{\circ}_{0}$, S°_{298}, $Cp^{\circ}_{298.15}$. The data from original sources have been ciritically evaluated by competent thermochemists and best values selected for the functions tabulated, maintaining internal consistency by the relationships $\Delta Gf^{\circ}_{298} = \Delta Hf^{\circ}_{298} - T\Delta S^{\circ}_{298}$, and $\Delta Hf^{\circ}_{298} = \Delta Hf^{\circ}_{0} = \Sigma (H^{\circ}_{298} - H^{\circ}_{0})$

25. Watt, B. K. and Merrill, A. L. (see Merrill, A. L. and Watt, B. K., source 12).

26. Wicks, C. E., and Block, F. E.

Thermodynamic Properties of 65 Elements - Their Oxides, Halides, Carbides, and Nitrides

Bureau of Mines Bulletin 605, (1963).

(U. S. Government Printing Office, Washington, D. C.)

Part I of this monograph is a seven page introduction to the application of thermodynamic functions, with particular reference to metallurgical process. Part II gives tabular data and graphs of enthalpy, enthalpy of formation, and Gibbs energy, for the substances listed in the title. Also listed are S_{298}, T_m, ΔH_m, T_b, ΔH_v, and analytic expressions for Cp, $H_T - H_{298}$, and $G_T - H_{298}$. The units are the calorie, the mole, and the kelvin. References to sources of information are given. The sources included original sources, reviews by other groups, and estimates. The data are, therefore, of very non-uniform reliability.

27. Wilhoit, R. C., and Zwolinski, B. J.

Handbook on Vapor Pressures and Heats of Vaporization of Hydrocarbons and Related Compounds (API 44 - TRC)

(Thermodynamics Research Center, Texas A and M Research Foundation, College Station, Texas, 1971)

This handbook gives subject data on 680 hydrocarbons, 95 sulfur compounds, and water from 0 to 150°C. It is indexed by compound name, and by boiling point.

28. Zemansky, M. W.

    Heat and Thermodynamics, 5th edition

    (McGraw Hill Book Company, New York, Etc., 1968)

This well known textbook provides a clear pedagogical presentation of the principal subjects of thermodynamics.

23.0 <u>Methods of Estimation of Thermodynamic Data</u>

Because of the essentially unlimited number of possible organic com-
pounds, and the very large number of inorganic compounds, the probability
of encountering a substance or material for which the thermodynamic pro-
perties have not been measured is quite large. Methods of estimation
are, therefore, essential to supplement tabulated values of thermodynamic
properties based on experimental studies. Some guides to the more com-
monly used methods are listed below. This is by no means a complete
list, as there have been some hundreds of studies of methods of correla-
tion or estimation.

1. American Society for Testing and Materials

    Estimation of Net Heat of Combustion of Aviation Fuels

    ASTM Method of Test D-1405

    ASTM Standards, Part 17, Petroleum Products

    (American Society for Testing and Materials, Philadelphia, Penn;

        annual)

This method of test allows an estimate accurate to about 0.5 percent
to be made of net heat of combustion of petroleum fuels having well de-
fined characteristics. Fuels included are certain classes of aviation
gasoline, jet engine fuels and kerosines. The required measurements are
aniline point and API gravity, which are routine laboratory tests applied
to most batches of petroleum products. The estimates have reduced valid-
ity if applied to fuels not meeting the specifications for which the
method was developed. The experimental studies and the correlations
were performed at the National Bureau of Standards.

2. American Society for Testing and Materials

    (1) Proposed Method for Estimation of Net and Gross Heat of

        Combustion of Burner and Diesel Fuels

        ASTM Standards, Part 17, Petroleum Products, January 1969,

        Appendix XI, D-2-1968

    (2) Proposed Method of Test for Estimation of Net Heat of

        Combustion of Distillate and Residual Fuels

        ASTM Standards on Petroleum Products, December 1962, Vol. I,

        Appendix XII, D-2-1962, pp. 1247-1259.

    (American Society for Testing and Materials, Philadelphia, Penna)

These tables, relating net and gross heat of combustion to API gravity of
diesel and burner fuels and distilled and residual fuels were published
for information by ASTM Committee D-2 on Petroleum Products and Lubri-
cants, but failed of acceptance as a standard method of test. The devia-
tions of individual actual fuels from the correlation and the disagreement
between these two sets of tables occurs principally in the very low API-
gravity range. The estimate of net heat of combustion may still be
expected to be valid to within a few percent. It is necessary to measure
API gravity in order to use this method for a particular batch of fuel.

3. Benson, S. W.

   Thermochemical Kinetics

   Methods for the Estimation of Thermochemical Data and Rate Parameters

   (John Wiley and Sons, Inc., New York, London, Sydney, 1968)

This monograph gives tables of necessary data and descriptions of methods
of their use for calculating ΔHf, Cp, and S, at 25°C for gas phase mole-

cules and radicals and for extrapolating them to higher temperatures. The
procedures can be applied to hydrocarbons, oxygen-containing compounds,
nitrogen-containing compounds, haloalkanes, organo-sulfur compounds, and
organo-metallic compounds; and deal principally with organic compounds.

4. Benson, S. W., Cruickshank, F. R., Golden, D. M., Haugen, G. R.,
    O'Neal, H. E., Rogers, A. S., Shaw, R., and Walsh, R.
    Additivity rules for the estimation of thermochemical properties.
    Chem. Rev. <u>69</u>, 279-324 (1969)

This lengthy technical article gives procedures for calculating the pro-
perties ΔHf°, S°, Cp°, for organic compounds in the gas phase. Parameters
for calculating Cp are given for temperatures from 300 to 1500 K at inter-
vals. The availability of Cp at T allows calculation of ΔHf° and S° at
the same temperatures. The necessary constants for making the calculations
are given for individual chemical groupings in some 38 tables. Many
classes of functional groups and molecular conformations are included.
Examples are given comparing calculated and observed values. Agreements
of 1 kcal mol^{-1} or less in ΔHf° and 1 cal mol^{-1} K^{-1} or less in Cp° and S°
are generally found.

5. Bondi, A.
    Physical Properties of Molecular Crystals, Liquids, and Glasses
    (John Wiley and Sons, Inc., New York, London, Sydney, 1968)

This monograph is designed for the use of chemical engineers to estimate
physical properties needed in design calculations, as well as of physical
chemists and synthetic chemists who need to understand the relationship
between structure and physical properties. Correlations of several kinds

are described in the text. These are then restated as methods for esti-
mation of the properties.

Substances considered include non-polar and polar gases, non-polar and
polar liquids, associated liquids, crystalline solids, glasses, polymers,
and polymer melts, as well as others. Procedures given include many
variants, depending upon the properties given as initial information.
Among the properties for which procedures are given are: density, heat
capacity, enthalpy, entropy, enthalpy and entropy of fusion, enthalpy of
sublimation and vapor pressure, cubical thermal expansion coefficient,
bulk modulus, Young's modulus, compressibility, thermal conductivity,
rotational diffusion constant, relaxation times, mass diffusion, vis-
cosity, and others.

6. Cox, J. D., and Pilcher, G.

    Thermochemistry of Organic and Organometallic Compounds

    (Academic Press, London, New York, 1970)

In this monograph, Chapter 7, "Some Theoretical Applications of
Thermochemical Data", gives a discussion of the application of schemes
for calculating ΔHf (or equally well, ΔHc).
The group-contribution method of Benson and Buss is discussed and tables
of group contributions are given. The bond-energy schemes (by which
ΔH (atomization) and hence ΔHf or ΔHc can be calculated) developed by
Laidler, and by Allen, are discussed and tables of contributing terms
are given. Other schemes developed by Tatevskii, Platt, Greenshields-
Rossini, and Somayajulu-Zwolinski, are briefly described. Special fac-
tors affecting these methods are discussed and illustrated including

steric effects, ring strain, and resonance. The accuracy of the estimates is discussed and examples of the use of the methods are given.

7. Janz, G. J.

Thermodynamic Properties of Organic Compounds

Estimation methods, principles and practice (revised edition)

(Academic Press, Inc., New York, London, 1967)

This well established monograph discusses computation of thermodynamic properties such as heat capacities, entropies, enthalpies and Gibbs energies by statistical mechanical methods, by methods of structural similarity, by methods of group contributions, by methods of group equations, and by methods of generalized vibrational assignments. The chemical properties: enthalpy of formation, and enthalpy of combustion are treated in terms of bond energies and group increments. Some 78 tables are given of increments, group contributions, and bond contributions as specifically needed for estimation of particular properties.

8. Joshi, R. M., and Zwolinski, B. J.

Vinyl Polymerization, Volume 1, Part I, edited by G. E. Ham

(Marcel Dekker, Inc., New York, 1967)

Chapter 8: Heats of Polymerization and their Structural and
            Mechanistic Implications

The application of various semi-empirical bond-energy schemes to the calculation of heats of polymerization are discussed.

9. Kubaschewski, O., Evans, E. Ll., and Alcock, C. B.

Metallurgical Thermochemistry, 4th edition

(Pergamon Press, Oxford, New York, and other cities, 1967)

This book contains a chapter of 35 pages on estimation of thermochemical
data. Methods are given for calculation of heat capacities (Cp) of
gases, solids, and liquids, and constants are given for estimating ΔCp
for some reactions involving gases. Estimation of entropies and enthal-
pies of evaporation and fusion is briefly treated. Tables and charts are
given for estimating entropies of solids and gases. Charts are given
illustrating regularities in enthalpies of formation of compounds, and
special attention is given to estimating enthalpies of formation of
inter-metallic compounds and sulfides, selenides, and tellurides.

10. Mason, D. M., and Eakin, B. E.

   Calculation of Heating Value and Specific Gravity of Fuel Gases

   Institute of Gas Technology Research Bulletin 32, (1961), 18 pp.

   (Institute of Gas Technology, Chicago, Illinois)

This pamphlet gives procedures for calculating heating value and specific
gravity of a gaseous fuel from an analysis of its component substances.
It is applicable to commercial fuel gases. Compressibility factors are
taken into account. The heating value calculation has errors less than
1%.

11. Pauling, L.

   The Nature of the Chemical Bond, 3rd edition

   (Cornell University Press, Ithaca, New York, 1960)

This well established monograph provides general information about the
nature of chemical binding in (principally) inorganic compounds which is
fundamentally very important for the estimation of enthalpies of forma-
tion, but not always easily applied.

12. Pitzer, K. S., and Brewer, L.

Thermodynamics: Gilbert N. Lewis and Merle Randall, 2nd edition

(McGraw Hill Book Co., New York, etc., 1961)

Chapter 32 of this book describes methods for estimating entropies and other thermodynamic properties. The emphasis is on entropy, but energies of inorganic substances are also briefly treated showing the use of a Born-Haber cycle. Ad hoc procedures are suggested for estimating enthalpies of formation of inorganic compounds for which data are not available.

13. Reid, Robert C., and Sherwood, T. K.

The Properties of Gases and Liquids, their Estimation and

   Correlation, 2nd edition.

(McGraw Hill Book Co., New York, etc., 1966)

This lengthy monograph follows the procedure of discussing various methods available for calculating or estimating particular properties of particular materials, and then provides recommendations for action with respect to each kind of property. Included in the book are procedures for making estimates of critical constants, normal boiling temperatures, Lennard-Jones-potential parameters, compressibility factors and equations of state, liquid molal volumes and densities, and vapor pressures. Estimates of enthalpies of vaporization, and of ideal-gas heat capacities, enthalpies and Gibbs energies of formation are treated. For real fluids variations of enthalpy, entropy, internal energy, and heat capacity with pressure are treated. Some methods are given for estimating the properties of fluid mixtures. Surface tension and the transport properties

--viscosity, diffusion coefficient and thermal conductivity--are discussed. Numerous tables present comparisons of observed and calculated properties.

14. Schafer, K., and Lax, E. (editors)

    Landolt-Börnstein

    Eigenschaften der Materie in Ihren Aggregatzustanden

    4 Teil. Kalorische Zustandgrossen, pp. 18-32

    (Springer-Verlag, Berlin, Gottingen, Heidelberg, 1961)

Extensive tables are given of group contributions to enthalpy of formation and Gibbs energy of formation of organic substances (gases) in kcal mol^{-1} and kJ mol^{-1}. They form a suitable basis for estimating properties of gases.

15. Tatevskii, V. M., Benderskii, V. A., and Yarovoi, S. S.

    Rules and Methods for Calculating the Physico-chemical Properties
      of Paraffinic Hydrocarbons

    (Translated from the Russian by M. F. Mullins and edited by B. P.
      Mullins)

    (Pergamon Press, New York, Oxford, London, Paris, 1961)

This monograph is a summary and a consolidation of the results of some years of work by Tatevskii and others, extending and elaborating some procedures introduced by Rossini and others. It suffers from ambiguity of statement which is somewhat distracting, but the methods presented in it have been attracting increasing attention recently. Properties calculated include: molar volume, molar refraction, vapor pressure, enthalpy of formation from atoms or elements, Gibbs energy of formation, and

enthalpy of combustion. Three different methods are used. Tables of

constants and illustrations of the accuracy of the methods are given.

24.0 Selected References on Combustion and High Temperature Reaction Equilibria

1. Bahn, Gilbert S., and Zukoski, Edward S., editors

    Kinetics, Equilibria, and Performance of High Temperature Systems.

    (Proceedings of the First Conference, 2-5 Nov., 1959)

    (Butterworths, Washington, D. C., 1960)

    This conference proceedings is directed primarily to rocket pro-
    pulsion systems and to chemical and phsycial processes occurring in
    propulsion systems. There are several papers describing procedures
    for calculating equilibria and temperatures of complex reacting systems.
    Several of these use digital computer programs which are described.
    See also proceedings of the second conference by the same title.

2. Berenblut, I. I., and Downes, A. B.

    Tables for Petroleum Gas - Oxygen Flames: Combustion Products and
       Thermodynamic Properties.

    (Oxford Press, New York and Oxford, 1960).

3. Bradley, J. N.

    Flame and Combustion Phenomena

    (Menthuen, Barnes & Noble, New York, 1969).

4. Combustion (Serial)

    (Combustion Publishing Co., Inc. New York, N. Y.)

5. Combustion and Flame (The Journal of the Combustion Institute)
    (Butterworths, London, 1957-)

    This journal publishes experimental and theoretical investigations
    dealing with combustion, detonation, and explosion, including such topics
    as: combustion in practical systems, fires, fluid dynamics, heat trans-
    fer and radiation; heterogeneous combustion; ignition; instability; mecha-
    nisms and kinetics; phase changes; thermal decomposition; thermochemistry
    and thermodynamics; and other topics.

6. Combustion Science and Technology (Serial)
    (Gordon and Breach, London, 1959-).

7. Corey, Richard C.
    Principles and Practice of Incineration
    (John Wiley and Sons, New York, N. Y., 1969).

8. Ducarme, J., Gerstein, M., and LeFebre, A. H., editors (Serial)
    Progress in Combustion Science and Technology
    (Pergamon Press, New York, 1961-).

9. Fleming, Donald K.
    Aerothermochemistry
    (First Biennial Gas Dynamics Symposium,1956)
    (Northwestern University Press, Evanston, Ill.).

10. Fristrom, R. M. and Westenberg, A. A.
    Flame Structure
    (McGraw-Hill Book Co., Inc., New York, N.Y., 1965).

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11. Gaydon, A. G., and Wolfhard, H. G.

    Flames, Their Structure, Radiation and Temperature

    (Chapman and Hall, Ltd., London, 1970).

12. Hougen, Olaf A., Watson, Kenneth M., and Ragatz, Roland R.

    Chemical Process Principles, Part II Thermodynamics

    (John Wiley and Sons, Inc., New York, N.Y.; Chapman & Hall,

     Ltd, London, 2nd ed. 1959).

    Chapter 25, "Chemical Equilibrium Constants, Chapter 26, "Equilibria
in Chemical Reactions," and Chapter 27, "Equilibria in Complex Reactions",
are of particular relevance to the determination of temperatures and
products of combustion resulting from combustion processes. Charts and
illustrative problems are given.

13. Jost, Wilhelm (H. O. Croft, translator)

    Explosion and Combustion Processes in Gases

    (McGraw-Hill Book Co., Inc., New York, N.Y., 1946).

14. Lewis, B., Pease, R. N., and Taylor, H. S. (editors)

    Combustion Processes

    (High Speed Aerodynamics and Jet Propulsion, Volume 2)

    (Princeton University Press, Princeton, N. J., 1956)

    In this large volume there are numerous chapters on the combustion
of solids, liquids, and gases, the kinetics of combustion reactions
and on detonation process by various authors. Chapter A by Carter and
Altman discusses reaction equilibrium and the temperatures obtained by
the combustion energy. Chapter C by S. R. Brinkley, Jr., discusses
computational methods for complex reacting systems.

15. Lewis, Bernard, and Von Elbe, G.

    Combustion, Flames and Explosions of Gases, 2nd ed.

    (Academic Press, New York, N. Y., 1961)

16. Minkoff, G. J. and Tippen, C.F.H.

    Chemistry of Combustion Reactions

    (Butterworths, London, 1962).

17. Mullins, B. P.

    Combustion Researches and Reviews, 1955

    (Pergamon Press, New York, 1955)

18. Mullins, B.P., and Fabri, J.

    Combustion Researches and Reviews, 1957

    (Pergamon Press, New York, N.Y., 1957)

19. Mullins, B. P., and Penner, S. S.

    Explosions, Detonations, Flammability and Ignition

    (Pergamon Press, New York, N.Y., 1962)

20. Penner, S. S.

    Chemistry Problems in Jet Propulsion

    (Pergamon Press, New York, N.Y., 1958)

21. Penner, S. S.

    Chemical Rocket Propulsion and Combustion Research

    (Gordon and Breach, New York, London, 1962)

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22. Penner, S. S., and Ducarme, J.

    Combustion and Propulsion Researches and Reviews, 1959

    The Chemistry of Propellants

    (Pergamon Press, New York, 1960)

23. Pugh, Brinley

    Fuel Calorimetry

    (Plenum Press, New York, N. Y., 1966)

24. Smith, Marion L., and Stinson, K. W.

    Fuels and Combustion

    (McGraw-Hill Book Company, New York, N. Y., 1952)

25. Spalding, D. B.

    Some Fundamentals of Combustion

    (Academic Press, Inc., New York, N.Y., 1955)

26. Starkman, Ernest S. (editor)

    Combustion Generated Air Pollution

    (Plenum Press, New York, London, 1971)

27. Strehlow, Roger A.

    Fundamentals of Combustion

    (International Textbook Company, Scranton, Pa., 1968)

28. Surugue, J. N.

    Experimental Methods in Combustion Research

    (Pergamon Press, New York, N.Y., 1960).

29. Symposium (International) on Combustion

     1st - 1928 to 12th - 1969

     (The Combustion Institute, Pittsburgh, Pa.)

30. Thring, M. W.

     Selected Combustion Problems

     (Pergamon Press, New York, N.Y.)

31. Thring, M. W.

     The Science of Flames and Furnaces

     (John Wiley & Sons, Inc., New York, 1952)

32. Thring, M. W., Fabri, J., Lutz, O., and Lefebre, A. H.

     Combustion and Propulsion - Third AGARD Colloquium

     (Pergamon Press, New York, N.Y., 1958)

33. Vulvis, L. A. (M. D. Friedman, translator)

     Thermal Regimes of Combustion

     (McGraw-Hill Book Co., Inc., New York, N.Y., 1961)

34. White, W. B., Johnson, S. M., and Dantzig, G. B.

     Chemical Equilibrium in Complex Mixtures

     J. Chem. Phys. $\underline{28}$, 751-755 (1958).

35. Wilkins, R. L.

     Theoretical Evaluation of Chemical Propellants

     (Prentice-Hall, Inc., Englewood Cliffs, N. J., 1963).

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36. Williams, Forman A.

Combustion Theory: The Fundamental Theory of Chemically

Reacting Flow Systems

(Addison-Wesley Publishing Co., Inc., Reading, Mass., Palo

Alto, Calif., London, 1965).

This is "an advanced graduate text or reference for workers in the field of combustion." Some sections deal specifically with processes occurring in rocket motors, but most of the text is so generally oriented that it is applicable to combustion problems in other areas. The titles of major sections are: Summary of basic fluid dynamics and chemical kinetics; Rankine-Hugoniot relations; Diffusion flames and droplet burning; Reactions in nozzle flow and in sound waves; Laminar flame theory; Gaseous detonations; Turbulent flames; Ignition, quenching, and flammability limits; Solid propellant deflagration; Combustion instability in solid and liquid propellant rockets; Monopropellant droplet burning; Spray combustion; Chemical reactions in boundary layers; Appendix A. Summary of applicable results of thermodynamics and statistical mechanics; Appendix B. Review of chemical kinetics; Appendix C. Continuum derivation of the conservation equations; Appendix D. Molecular derivation of the continuum equations; Appendix E. Transport properties.

37. Wolfhard, H. G., Classman, I., and Green, L., Jr. (editors)

Heterogeneous Combustion

(Progress in Astronautics and Aeronautics, Vol. 15)

(Academic Press, Inc., New York, N.Y., 1965).

38. Zabetakis, M. G.

    Flammability Characteristics of Combustible Gases and Vapors

    (Bureau of Mines Bulletin 627, 1965).

39. Zeleznik, F. J., and Gordon, S.

    A General IBM 704 or 7090 Computer Program for Computation

      of Chemical Equilibrium Compositions, Rocket Performance,

      and Chapman-Jouguet Detonations

    NASA TN D-1454 (October 1962).

      See also NASA TN D-132 (October, 1959)

          and NASA TN D-1737 (October, 1963).

25.0 Tables of Thermodynamic Data

25.1 Description of the Tables

Table I-A Enthalpies of Formation of Some Organic Compounds

and Inorganic Carbon Compounds at 298.15 K.

Content. Table I-A is a list of about 1000 carbon compounds (989 compounds, some differing in physical state or stereochemical configuration gave a total of 1093 entries) in which the information given in columns, left to right, is: molecular formula, formula weight, name (physical state), enthalpy (heat) of formation in kcal mol^{-1}, enthalpy (heat) of formation in kJ mol^{-1}, references for enthalpy data.

Formula format. A molecular formula (for substances consisting of discrete molecules) is given in which the elements are listed in a partially alphabetical order with the numbers of atoms as subscripts. Carbon is always the first element. Hydrogen, if present, is always the second element. The remaining elements follow in the alphabetical order of their chemical symbols. Empirical formulas are given for ionic solids.

Arrangement of compounds. The formulas are listed in alphabetical order following the arrangement of the Chemical Abstracts Formula Index (Hill arrangement, E. A. Hill, J. Am. Chem. Soc. 22, 478-494 (1900)). The compounds are also in numerical order of the number of atoms per molecule. Beginning with the element on the left, the lowest subscripts are listed first and increase to higher numbers only when all elements

to the right have been listed from the lowest to the highest number.
Thus, all compounds with C_1 are listed before any with C_2; all compounds
with C_1A_1 before any with C_1A_2, and so on. The arrangement is illustrated
in figure 25.1.
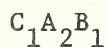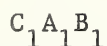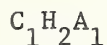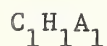
C_1A_1

$C_1A_1B_1$

C_1A_2 Figure 25.1

$C_1A_2B_1$ alphabetic-numeric

C_1H_1 arrangement of compounds

$C_1H_1A_1$

C_1H_2

$C_1H_2A_1$

C_1Z_1

C_1Z_2

C_2A_1

Compound name (and physical state). A well known name for each
compound is given to make a positive identification of the substance
and remove any ambiguity resulting from the possibility of several
isomeric forms having the same composition and molecular weight. The
physical state of the compound is listed: gas (g), Liquid (liq), or
crystal (c).

Enthalpy of formation. (Sometimes called heat of formation). The enthalpy of formation of the compound from the elements is given in two columns, respectively in kilocalories per mole and in kilojoules per mole. In the table of data the uncertainties are not given explicitly. The values in general are accurate to between one and 10 parts in the last figure given. A negative enthalpy of formation means the reaction of formation from the elements is exothermic.

Reference. The values of enthalpies of formation were taken from a few collections of carefully evaluated data and represent the best current appraisal of the available experimental data. The source references are listed at the end of the table.

Table I-B Compound Name-Formula Index (of Carbon Compounds)

Content. Table I-B is a name-formula index of all the compounds in Table I-A arranged alphabetically in order of the name. For some compounds, an alternative name is listed with a cross reference to the name found in Table I-A.

Use of Table I - To find the enthalpy (heat) of formation of a compound.
Write the molecular formula of the compound in the format given in paragraph 2 above, and then look for the formula in Table I-A following the arrangement listed in paragraph 3 above. Some formulas represent more than one substance. Distinguish between them by the name and physical state.

If the formula is not known, look up the name in the alphabetical listing in Table I-B to find the formula, and then proceed as before. Failure to find the name in the alphabetical listing does not mean for

sure that the compound is not listed, as it has been impossible to list all the names that may be used for the compounds. In event the compound is not found in the alphabetical name index, look for alternate names, or determine the formula and proceed as above.

Table II - Enthalpies of Formation of Organic Polymers at 298.15 K.

Content. Table II is a list of 39 organic polymers, in which the information given in columns, left to right is: chemical formula of the repeating unit, formula weight of the repeating unit, name (and physical state), enthalpy (heat) of formation in kcal mol^{-1}, enthalpy (heat) of formation in kJ mol^{-1}, references for enthalpy data.

Formula format. Same as Table I-A.

Arrangement of Compounds. Same as Table I-A.

Compound name, (and physical state). A name based on the monomer is frequently given. A few common names and trade names are used.

Enthalpy (heat) of formation. The value cited represents the enthalpy of formation of the repeating unit from the elements. Uncertainties are not explicitly given. The values, in general, are accurate to between one and ten parts in the last figure given.

Reference. The original source of the heat of combustion data is given. A list of references is found at the end of the table.

Table III - Enthalpies of Formation of Inorganic Oxides at 298.15 K.

Content. Table III is a list of 285 inorganic oxides, in which the information given in columns, left to right is: empirical or molecular formula (and physical state), formula weight, name, enthalpy

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(heat) of formation in kcal mol^{-1}, enthalpy (heat) of formation in kJ mol^{-1}, reference for enthalpy data.

Formula format. Solids forming continuous covalent or ionic lattices have the empirical formula given. Gases, liquids, or solids having molecules (as for instance As_4O_6(c)) are represented as the molecular formula. Oxygen is listed last in the formula. The state: gas (g), liquid (liq), or solid (c) is listed in parenthesis following the formula. When more than one crystal form is known, the crystal form is listed. Non-crystalline solids are listed as amorphous (amorph).

Arrangement of compounds. The formulas are listed in alphabetical order of the symbol of the first element and in order of increasing numbers of atoms of each element in the formula. Phases of the same compound are listed in the order (g), (liq), (c).

Compound name. A descriptive chemical name is given. In a few cases a common synonym or a mineral name is given.

Enthalpy of formation. (Sometimes called heat of formation). The enthalpy of formation from the elements is given in two columns, respectively in kilocalories per mole, and kilojoules per mole. In the table the uncertainties are not given explicitly. The values in general are accurate to between one and ten parts in the last figure given. A negative enthalpy of formation means the reaction of formation from the elements is exothermic.

Reference. Numerical references refer to the source of the data in the list of references at the end of the table. All data were taken from reliable collections of carefully evaluated data and represent the best current appraisal of the available experimental data.

25.2 TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	Formation kJ mol^{-1}	Ref
CAg_2O_3	275.7494	Silver carbonate (c)	-120.9	-505.8	(3)
$CBrF_3$	148.9154	Bromotrifluoromethane (g)	-153.6	-642.7	(2)
CBr_2O	187.8286	Carbonyl dibromide (g)	-23.0	-96.2	(2)
CBr_2O	187.8286	Carbonyl dibromide (liq)	-30.4	-127.2	(2)
CBr_3	251.7382	Carbon tribromide (g)	+42.	+176.	(2)
CBr_4	331.6472	Carbon tetrabromide (g)	+19.	+79.	(2)
CBr_4	331.6472	Carbon tetrabromide (c)	+4.5	+18.8	(2)
$CClF_3$	104.4594	Chlorotrifluoromethane (g)	-166.	-695.	(2)
CCl_2F_2	120.9140	Dichlorodifluoromethane (g)	-114.	-477.	(2)
CCl_2O	98.9166	Carbonyl dichloride (g)	-52.3	-218.8	(2)
CCl_3	118.3702	Carbon trichloride (g)	+14.	+59.	(2)
CCl_3F	137.3686	Fluorotrichloromethane (g)	-66.	-275.	(2)
CCl_3F	137.3686	Fluorotrichloromethane (liq)	-72.02	-301.33	(2)
CCl_4	153.8232	Carbon tetrachloride (g)	-24.6	-102.9	(2)
CCl_4	153.8232	Carbon tetrachloride (liq)	-32.37	-135.44	(2)
$CCoO_3$	118.9426	Cobalt carbonate (c)	-170.4	-713.0	(3)
CF_2O	66.0074	Carbonyl difluoride (g)	-151.7	-634.7	(2)
CF_3	69.0064	Carbon trifluoride (g)	-114.	-477.	(2)
CF_4	88.0048	Carbon tetrafluoride (g)	-223.0	-933.0	(2)
$CFeO_3$	115.8564	Iron (II) carbonate (c)	-177.00	-740.57	(3)
$CHBr_3$	252.7461	Bromoform (g)	+4.	+17.	(2)
$CHBr_3$	252.7461	Bromoform (liq)	-6.8	-28.5	(2)
$CHCl_3$	119.3781	Chloroform (g)	-24.65	-103.4	(2)
$CHCl_3$	119.3781	Chloroform (liq)	32.14	-134.47	(2)
CHF_3	70.0143	Fluoroform (g)	-164.5	-688.3	(2)
CHI_3	393.7323	Iodoform (c)	+33.7	+141.0	(2)
CH_2Cl_2	84.9331	Methylene dichloride (g)	-22.10	-92.47	(2)
CH_2Cl_2	84.9331	Methylene dichloride (liq)	-29.03	-121.46	(2)
CH_2F_2	52.0239	Methylene difluoride (g)	-106.8	-446.9	(2)
CH_2I_2	267.8359	Methylene diiodide (g)	+27.0	+113.0	(2)
CH_2I_2	267.8359	Methylene diiodide (liq)	+16.0	+56.9	(2)
CH_2N_4	70.0539	Tetrazole (c)	+56.7	+237.2	(1)
CH_2N_4O	86.0533	5-Hydroxytetrazole (c)	+1.5	+5.3	(1)
CH_2O	30.0265	Formaldehyde (g)	-25.95	-108.57	(1)
CH_2O_2	46.0259	Formic acid (liq)	-101.51	-424.72	(1)
CH_3BO	41.8455	Carbonyl borane (g)	-26.58	-111.21	(2)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 299.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	Enthalpy of Formation kJ mol^{-1}	Ref
CH_3Br	94.9441	Methyl bromide (g)	-8.4	-35.1	(2)
CH_3Cl	50.4881	Methyl chloride (g)	-19.32	-80.83	(2)
CH_3Hg	215.6251	Methyl mercury (g)	+40.	+167.	(3)
CH_3I	141.9395	Methyl iodide (g)	+3.1	+13.0	(2)
CH_3I	141.9395	Methyl iodide (liq)	-3.7	-15.5	(2)
CH_3NO	45.0412	Formamide (liq)	-60.7	-254.0	(1)
CH_3N_5	85.0686	5-Aminotetrazole (c)	+49.7	+207.9	(1)
CH_3OTl	235.4045	Thallium methoxide (c)	-27.5	-115.1	(2)
CH_4	16.0430	Methane (g)	-17.89	-74.85.	(1)
CH_4N_2O	60.0558	Urea (c)	-79.71	-333.51	(1)
CH_4N_2S	76.1204	Thiourea (c)	-21.13	-88.41	(1)
$CH_4N_6O_3$	148.0814	5-Aminotetrazole nitrate (c)	-6.6	-27.6	(1)
CH_4O	32.0424	Methanol (g)	-47.96	-200.66	(1)
CH_4O	32.0424	Methanol (liq)	-57.04	-238.66	(1)
CH_4S	48.1070	Methanethiol (liq)	-11.08	-46.36	(1)
CH_5N	31.0577	Methylamine (liq)	-11.3	-47.3	(1)
CH_5N_3	59.0711	Guanidine (c)	-13.39	-56.02	(1)
$CH_5N_3O_4$	123.0687	Urea nitrate (c)	-134.8	-564.0	(1)
$CH_5N_5O_2$	119.0833	Nitroaminoguanidine (c)	+5.29	+22.13	(1)
$CH_6N_2O_3$	94.0706	Methylamine nitrate (c)	-84.7	-354.4	(1)
$CH_6N_4O_3$	122.0840	Guanidine nitrate (c)	-92.5	-387.0	(1)
$CH_8N_6O_3$	152.1133	sym-Diaminoguanidine nitrate (c)	-37.57	-157.19	(1)
$CMnO_3$	114.9474	Manganese carbonate, natural (c)	-213.7	-894.1	(3)
$CMnO_3$	114.9474	Manganese carbonate, precipitated (c)	-211.1	-883.2	(3)
CO_3Tl_2	468.7494	Thallium carbonate (c)	-167.3	-700.0	(2)
CO_3Zn	125.3794	Zinc carbonate (c)	-194.26	-812.78	(2)
$C_2Ag_2O_4$	303.7599	Silver oxalate (c)	-160.9	-673.2	(3)
$C_2Br_2F_4$	259.8339	1,2-Dibromo-1,1,2,2-tetrafluoroethane(g)	-186.5	-780.3	(2)
C_2Cd0_4	200.4199	Cadmium oxalate (c)	-218.1	-912.5	(2)
C_2ClF_3	116.4705	Chlorotrifluoroethylene (g)	-132.7	-555.2	(2)
$C_2Cl_2F_2$	132.9251	1,2-Dichloro-1,2-difluoroethylene (g)	-76.3	-319.2	(2)
$C_2Cl_2F_4$	170.9219	1,1,2,2-Tetrafluoro-1,2-dichloroethane(g)	-212.8	-890.4	(2)
$C_2Cl_3F_3$	187.3765	1,1,2-Trichloro-2,2,1-trifluoroethane (g)	-181.5	-759.4	(2)
$C_2Cl_3F_3$	187.3765	1,1,2-Trichloro-2,2,1-trifluoroethane (liq)	-188.37	-788.16	(2)
C_2Cl_4	165.8343	Tetrachloroethylene (g)	-2.9	-12.1	(2)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	Formation kJ mol⁻¹	Ref
C_2Cl_4	165.8343	Tetrachloroethylene (liq)	-12.5	-52.3	(2)
$C_2Cl_4F_2$	203.8311	1,1,1,2-Tetrachloro-2,2-difluoroethane (g)	-117.1	-489.9	(2)
C_2Cl_4O	181.8337	Trichloroacetyl chloride (liq)	-66.65	-278.96	(2)
C_2Cl_6	236.7403	Hexachloroethane (c,I)	-46.0	-192.5	(2)
C_2Cl_6	236.7403	Hexachloroethane (c,II)	-47.9	-200.4	(2)
C_2Cl_6	236.7403	Hexachloroethane (c,III)	-48.5	-202.9	(2)
C_2Cl_6	236.7403	Hexachloroethane (g)	-33.9	-141.9	(2)
C_2CoO_4	146.9531	Cobalt oxulate (c)	-203.5	-851.4	(3)
C_2F_4	100.0159	Tetrafluoroethylene (g)	-155.5	-650.6	(2)
C_2F_6	138.0127	Hexafluoroethane (g)	-310.	-1297.	(2)
$C_2HBrCl_2F_2$	213.8421	1-Bromo-1,1-difluoro-2,2-dichloroethane (g)	-107.9	-451.5	(2)
C_2HBrF_4	180.9329	1,1,2,2-Tetrafluorobromoethane (g)	-197.0	-824.2	(2)
C_2HBr_3O	280.7567	Bromal (liq)	-31.13	-130.25	(2)
C_2HClF_2	98.4801	1,1-Difluoro-2-chloroethylene (g)	-75.4	-315.5	(2)
C_2HCl_3	131.3893	Trichloroethylene (g)	-1.86	-7.78	(2)
C_2HCl_3	131.3893	Trichloroethylene (liq)	-10.1	-42.3	(2)
C_2HCl_3O	147.3887	Chloral (g)	-47.0	-196.6	(2)
C_2HCl_3O	147.3887	Chloral (liq)	-56.45	-236.19	(2)
C_2HCl_3O	147.3887	Dichloroacetyl chloride (liq)	-67.27	-281.46	(2)
$C_2HCl_3O_2$	163.3881	Trichloroacetic acid (c)	-120.7	-505.0	(2)
C_2HCl_5	202.2953	Pentachloroethane (liq)	-44.9	-187.9	(2)
C_2HN_5	95.0638	5-Cyanotetrazole (c)	+96.1	+402.1	(1)
C_2H_2	26.0382	Acetylene (g)	+54.19	+226.73	(1)
$C_2H_2Br_2Cl_2$	256.7622	1,2-Dibromo-1,2-dichloroethane (g)	-8.8	-36.8	(2)
$C_2H_2Cl_2$	96.9442	1,1-Dichloroethylene (g)	+0.58	+2.43	(2)
$C_2H_2Cl_2$	96.9442	1,1-Dichloroethylene (liq)	-5.8	-24.3	(2)
$C_2H_2Cl_2$	96.9442	cis-1,2-Dichloroethylene (g)	+0.9	+3.9	(2)
$C_2H_2Cl_2$	96.9442	cis-1,2-Dichloroethylene (liq)	-6.6	-27.6	(2)
$C_2H_2Cl_2$	96.9442	trans-1,2-Dichloroethylene (g)	+1.47	+6.15	(2)
$C_2H_2Cl_2$	96.9442	trans-1,2-Dichloroethylene (liq)	-5.53	-23.14	(2)
$C_2H_2Cl_2O$	112.9436	Chloroacetyl chloride (liq)	-67.85	-283.68	(2)
$C_2H_2Cl_2O_2$	128.9430	Dichloroacetic acid (liq)	-119.0	-497.9	(2)
$C_2H_2Cl_4$	167.8502	1,1,2,2-Tetrachloroethane (g)	-35.7	-149.4	(2)
$C_2H_2Cl_4$	167.8502	1,1,2,2-Tetrachloroethane (liq)	-47.0	-196.6	(2)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	Enthalpy of Formation kJ mol⁻¹	Ref
$C_2H_2CoO_4$	148.9690	Cobaltous formate (c)	-208.7	-873.2	(3)
$C_2H_2CuO_4$	153.5758	Copper (II) formate (c)	-186.7	-781.2	(3)
$C_2H_2F_2$	64.0350	1,1-Difluoroethylene (g)	-78.6	-328.9	(2)
$C_2H_2F_2O_2$	96.0338	Difluoroacetic acid (liq)	-207.8	-869.4	(2)
$C_2H_2MnO_4$	144.9738	Manganese formate (c)	-249.7	-1044.7	(3)
$C_2H_2N_6$	110.0784	3-Azido-s-triazole (c)	+105.5	+441.4	(1)
$C_2H_2NiO_4$	148.7458	Nickel formate (c)	-208.4	-871.9	(3)
$C_2H_2O_2$	58.0370	Glyoxal (g)	-50.66	-211.96	(1)
$C_2H_2O_4$	90.0358	Oxalic acid (c,α)	-197.7	-827.2	(1)
$C_2H_2O_4$	90.0358	Oxalic acid (c,β)	-197.4	-825.9	(1)
$C_2H_2O_4Pb$	297.2258	Lead formate (c)	-210.0	-878.6	(2)
$C_2H_2O_4Zn$	155.4058	Zinc formate (c)	-235.8	-986.6	(2)
$C_2H_3AgO_2$	166.9150	Silver acetate (c)	-95.3	-398.7	(3)
C_2H_3Br	106.9552	Vinyl bromide (g)	+18.7	+78.2	(2)
C_2H_3BrO	122.9546	Acetyl bromide (liq)	-53.39	-223.39	(2)
$C_2H_3Br_3O_2$	298.7720	Bromal hydrate (c)	-112.	-469.	(2)
C_2H_3Cl	62.4992	Vinyl chloride (g)	+8.5	+35.6	(2)
C_2H_3Cl	62.4992	Vinyl chloride (liq)	+3.5	+14.6	(2)
C_2H_3ClO	78.4986	Acetyl chloride (g)	-58.20	-243.51	(2)
C_2H_3ClO	78.4986	Acetyl chloride (liq)	-65.44	-273.80	(2)
C_2H_3ClO	78.4986	Monochloroacetaldehyde (liq)	-61.5	-257.3	(2)
$C_2H_3ClO_2$	94.4980	Monochloroacetic acid (c,I)	-122.3	-511.7	(2)
$C_2H_3ClO_2$	94.4980	Monochloroacetic acid (c,II)	-122.12	-510.95	(2)
$C_2H_3ClO_2$	94.4980	Monochloroacetic acid (c,III)	-121.46	-508.19	(2)
$C_2H_3Cl_3$	133.4052	1,1,2-Trichloroethane (g)	-33.94	-142.00	(2)
$C_2H_3Cl_3$	133.4052	1,1,2-Trichloroethane (liq)	-43.5	-182.0	(2)
$C_2H_3Cl_3O_2$	165.4040	Chloral hydrate (c)	-137.7	-576.1	(2)
$C_2H_3Cl_3O_2$	165.4040	Chloral hydrate (g)	-107.2	-448.5	(2)
C_2H_3FO	62.0440	Acetyl fluoride (g)	-104.9	-438.9	(2)
C_2H_3FO	62.0440	Acetyl fluoride (liq)	-110.83	-463.71	(2)
$C_2H_3FO_2$	78.0434	Fluoroacetic acid (c)	-164.5	-688.3	(2)
$C_2H_3F_3$	84.0414	1,1,1-Trifluoroethane (g)	-176.0	-736.4	(2)
$C_2H_3F_3$	84.0414	1,1,2-Trifluoroethane (g)	-174.7	-730.9	(2)
$C_2H_3F_3O$	100.0408	2,2,2-Trifluoroethanol (liq)	-205.4	-859.4	(2)
C_2H_3IO	169.9500	Acetyl iodide (liq)	-38.84	-162.51	(2)
$C_2H_3NO_3$	89.0511	Oxamic acid (c)	-160.4	-671.1	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	Formation kJ mol^{-1}	Ref
$C_2H_3N_7$	125.0931	4-Amino-3-azido-s-triazole (c)	+136.5	+571.1	(1)
$C_2H_3O_2Tl$	263.4150	Thallium acetate (c)	-126.1	-527.6	(2)
C_2H_4	28.0542	Ethylene (g)	+12.50	+52.30	(1)
C_2H_4BrI	234.8676	1-Bromo-2-iodoethane (c)	-11.3	-47.3	(2)
$C_2H_4Br_2$	187.9722	1,2-Dibromoethane (g)	-9.16	-38.33	(2)
$C_2H_4Br_2$	187.8722	1,2-Dibromoethane (liq)	-19.4	-81.4	(2)
$C_2H_4Cl_2$	98.9602	1,1-Dichloroethane (g)	-30.93	-129.41	(2)
$C_2H_4Cl_2$	98.9602	1,1-Dichloroethane (liq)	-38.3	-160.2	(2)
$C_2H_4Cl_2$	98.9602	1,2-Dichloroethane (g)	-31.02	-129.79	(2)
$C_2H_4Cl_2$	98.9602	1,2-Dichloroethane (liq)	-39.49	-165.23	(2)
$C_2H_4F_2$	66.0510	1,1-Difluoroethane (g)	-114.3	-478.2	(2)
$C_2H_4F_2O$	82.0504	2,2-Difluoroethanol (liq)	-164.8	-689.5	(2)
$C_2H_4I_2$	281.8630	1,2-Diiodoethane (c)	+0.1	+0.4	(2)
$C_2H_4I_2$	281.8630	1,2-Diiodoethane (g)	+15.9	+66.5	(2)
$C_2H_4N_2O_2$	88.0664	Formylurea (c)	-118.	-494.	(1)
$C_2H_4N_2O_2$	88.0664	Oxamide (c)	-123.0	-514.6	(1)
$C_2H_4N_4$	84.0810	3-Amino-1,2,4-triazole (c)	+18.4	+77.0	(1)
$C_2H_4N_4O$	100.0804	5-Methoxytetrazole (c)	+16.6	+69.4	(1)
$C_2H_4N_4O_2$	116.0798	Azodicarbamide (c)	-69.90	-292.46	(1)
$C_2H_4N_{10}$	168.1212	5,5'-Hydrazotetrazole (c)	+135.1	+565.3	(1)
C_2H_4O	44.0536	Acetaldehyde (g)	-39.72	-166.19	(1)
C_2H_4O	44.0536	Acetaldehyde (liq)	-45.96	-192.30	(1)
C_2H_4OS	76.1176	Thiolacetic acid (liq)	-52.39	-219.20	(1)
$C_2H_4O_2$	60.0530	Acetic acid (liq)	-115.71	-484.13	(1)
$C_2H_4O_2$	60.0530	Methyl formate (g)	-83.7	-350.2	(1)
$C_2H_4O_2$	60.0530	Methyl formate (liq)	-90.6	-379.1	(1)
$C_2H_4O_3$	76.0524	Glycolic acid (c)	-158.6	-663.6	(1)
$C_2H_4O_4$	92.0518	Glyoxylic acid (c)	-199.7	-835.5	(1)
C_2H_4S	60.1182	Thiacyclopropane (liq)	+12.41	+51.92	(1)
C_2H_5Br	108.9712	Ethyl bromide (g)	-15.42	-64.52	(2)
C_2H_5Br	108.9712	Ethyl bromide (liq)	-21.99	-92.01	(2)
C_2H_5Cl	64.5152	Ethyl chloride (g)	-26.81	-112.17	(2)
C_2H_5Cl	64.5152	Ethyl chloride (liq)	-32.63	-136.52	(2)
C_2H_5ClO	80.5146	Ethylene chlorohydrin (liq)	-70.6	-295.4	(2)
C_2H_5FO	64.0600	2-Fluoroethanol (liq)	-111.3	-465.7	(2)
C_2H_5I	155.9666	Ethyl iodide (g)	-1.84	-7.70	(2)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	Enthalpy of Formation kJ mol^{-1}	Per
C$_2$H$_5$I	155.9666	Ethyl iodide (liq)	-9.6	-40.2	(2)
C$_2$H$_5$N	43.0689	Ethylenimine (liq)	+21.97	+91.92	(1)
C$_2$H$_5$NO	59.0683	Acetamide (c)	-76.0	-318.0	(1)
C$_2$H$_5$NO$_2$	75.0677	Glycine (c)	-126.22	-528.10	(1)
C$_2$H$_5$N$_5$	99.0957	1-Methyl-5-aminotetrazole (c)	+46.25	+193.51	(1)
C$_2$H$_5$N$_5$	99.0957	2-Methyl-5-aminotetrazole (c)	+50.4	+210.9	(1)
C$_2$H$_5$N$_5$	99.0957	5-Methylaminotetrazole (c)	+48.4	+202.5	(1)
C$_2$H$_5$N$_5$O$_3$	147.0939	3-Amino-1,2,4-triazole nitrate (c)	-40.9	-171.1	(1)
C$_2$H$_5$N$_5$O$_3$	147.0939	1-Formamido-2-nitroguanidine (c)	-35.1	-146.9	(1)
C$_2$H$_5$N$_7$	127.1091	5-Guanylaminotetrazole (c)	+40.5	+169.5	(1)
C$_2$H$_5$OTl	249.4316	Thallium ethoxide (liq)	-56.5	-236.4	(2)
C$_2$H$_6$	30.0701	Ethane (g)	-20.24	-84.68	(1)
C$_2$H$_6$Cd	142.7401	Dimethyl cadmium (g)	+24.27	+101.55	(2)
C$_2$H$_6$Cd	142.4701	Dimethyl cadmium (liq)	+15.2	+53.6	(2)
C$_2$H$_6$Hg	230.6601	Dimethyl mercury (g)	+22.56	+94.39	(3)
C$_2$H$_6$Hg	230.6601	Dimethyl mercury (liq)	+14.3	+59.8	(3)
C$_2$H$_6$N$_2$O$_5$	138.0805	Glycine nitrate (c)	-174.1	-728.4	(1)
C$_2$H$_6$N$_4$O$_2$	118.0957	Hydrazodicarbamide (c)	-119.19	-498.69	(1)
C$_2$H$_6$O	46.0695	Dimethyl ether (g)	-43.99	-184.05	(1)
C$_2$H$_6$O	45.0695	Ethanol (g)	-56.19	-235.10	(1)
C$_2$H$_6$O	46.0695	Ethanol (liq)	-66.37	-277.69	(1)
C$_2$H$_6$O$_2$	62.0689	1,2-Ethanediol (liq)	-108.70	-454.80	(1)
C$_2$H$_6$O$_6$	126.0665	Oxalic acid dihydrate (c)	-341.0	-1426.7	(1)
C$_2$H$_6$S	62.1341	Ethanethiol (liq)	-17.53	-73.35	(1)
C$_2$H$_6$S	62.1341	2-Thiapropane (liq)	-15.55	-65.06	(1)
C$_2$H$_6$S$_2$	94.1981	2,3-Dithiabutane (liq)	-14.82	-62.01	(1)
C$_2$H$_6$S$_2$	94.1981	1,2-Ethanedithiol (liq)	-12.83	-53.63	(1)
C$_2$H$_6$Si	58.1561	Vinylsilane (g)	-2.	-8.	(2)
C$_2$H$_6$Zn	95.4401	Dimethyl zinc (g)	+12.67	+53.01	(2)
C$_2$H$_6$Zn	95.4401	Dimethyl zinc (liq)	+5.6	+23.4	(2)
C$_2$H$_7$BO$_2$	73.8379	Dimethoxyborane (g)	-138.5	-579.5	(2)
C$_2$H$_7$BO$_2$	73.8879	Dimethoxyborane (liq)	-144.7	-605.4	(2)
C$_2$H$_7$N	45.0843	Dimethylamine (liq)	-10.5	-43.9	(1)
C$_2$H$_7$N	45.0843	Ethylamine (liq)	-17.7	-74.1	(1)
C$_2$H$_7$NO$_3$S	125.1470	2-Aminoethane-1-sulfonic acid (c)	-187.7	-785.3	(1)
C$_2$H$_7$N$_5$O$_4$	165.1092	Guanylurea nitrate (c)	-102.1	-427.2	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	kJ mol⁻¹	Ref
$C_2H_8N_2$	60.0995	Ethylenediamine (liq)	-15.06	-63.01	(1)
$C_2H_8N_2O_3$	108.0977	Dimethylamine nitrate (c)	-79.6	-333.0	(1)
$C_2H_8N_2O_3$	108.0977	Ethylamine nitrate (c)	-87.7	-366.9	(1)
C_2H_8Sn	150.7761	Dimethyl tin (g)	+21.	+88.	(2)
C_2H_8Sn	150.7761	Dimethyl tin (liq)	+14.5	+60.7	(2)
$C_2H_8N_{10}O$	188.1525	1-(5-Tetrazoyl)-4-guanyltetrazene monohydrate (c)	+45.2	+189.1	(1)
$C_2H_{10}N_4O_6$	186.1252	Ethylenediamine dinitrate (c)	-156.2	-653.5	(1)
C_2I_4	531.6399	Tetraiodoethylene (c)	+73.	+305.	(2)
C_2NIO_4	146.7299	Nickel oxalate (c)	-204.8	-856.9	(3)
$C_3H_2N_2O_3$	114.0610	Parabanic acid (c)	-138.0	-577.4	(1)
C_3H_4	40.0653	Propadiene (g)	+45.93	+192.17	(4)
C_3H_4	40.0653	Propyne (g)	+44.33	+185.48	(4)
$C_3H_4N_2$	68.0787	Imidazole (c)	+14.5	+60.7	(1)
$C_3H_4N_2$	68.0787	Pyrazole (c)	+28.3	+118.4	(1)
$C_3H_4N_2OS$	116.1421	Thiohydantoin (c)	-59.5	-248.9	(1)
$C_3H_4N_2O_2$	100.0775	Hydantoin (c)	-107.2	-448.5	(1)
$C_3H_4N_6$	124.1055	3-Azido-5-methyl-s-triazole (c)	+93.8	+392.5	(1)
$C_3H_4O_2$	72.0641	Acrylic acid (liq)	-91.8	-384.1	(1)
$C_3H_4O_2$	72.0641	β-Propiolactone (g)	-67.61	-282.88	(1)
$C_3H_4O_2$	72.0641	β-Propiolactone (liq)	-78.85	-329.91	(1)
$C_3H_4O_3$	88.0635	Ethylene carbonate (c)	-138.9	-581.2	(1)
$C_3H_4O_3$	88.0635	Pyruvic acid (c)	-140.3	-587.0	(1)
$C_3H_4O_4$	104.0629	Malonic acid (c)	-212.96	-891.02	(1)
$C_3H_4O_6$	136.0617	Mesoxalic acid (c)	-290.7	-1216.3	(1)
$C_3H_5N_5O$	127.1062	5-Acetamidotetrazole (c)	-1.2	-5.0	(1)
$C_3H_5N_7$	139.1202	4-Amino-3-azido-5-methyl-s-triazole (c)	+115.6	+483.7	(1)
C_3H_6	42.0813	Cyclopropane (g)	+12.75	+53.35	(1)
C_3H_6	42.0813	Propene (g)	+4.89	+20.46	(4)
$C_3H_6N_2O_2$	102.0935	Malonamide (c)	-130.5	-546.0	(1)
$C_3H_6N_2O_2S$	134.1575	Thiohydantoic acid (c)	-132.6	-554.8	(1)
$C_3H_6N_2O_3$	118.0929	Hydantoic acid (c)	-179.	-749.	(1)
$C_3H_6N_4$	98.1081	1,5-Dimethyltriazole (c)	+45.1	+188.7	(1)
$C_3H_6N_4O$	114.1075	1,4-Dimethyl-5-tetrazolone (c)	-6.6	-27.6	(1)
$C_3H_6N_6$	126.1215	Melamine (c)	-17.3	-72.4	(1)
C_3H_6O	58.0807	Oxacyclobutane (g)	-19.25	-80.54	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of kcal mol^{-1}	Formation kJ mol^{-1}	Ref
C$_3$H$_6$O	58.0807	Propanone (g)	-51.78	-216.55	(1)
C$_3$H$_6$O	58.0807	Propanone (liq)	-59.18	-247.61	(1)
C$_3$H$_6$O	58.0807	n-Propionaldehyde (liq)	-53.0	-221.8	(1)
C$_3$H$_6$O$_2$	74.0801	Methyl acetate (liq)	-106.4	-445.2	(1)
C$_3$H$_6$O$_2$	74.0801	Propionic acid (liq)	-122.07	-510.74	(1)
C$_3$H$_6$O$_2$S	106.1441	β-Thiolactic acid (liq)	-111.6	-466.9	(1)
C$_3$H$_6$O$_3$	90.0795	Glyceraldehyde (liq)	-143.	-598.	(1)
C$_3$H$_6$O$_3$	90.0795	D-Lactic acid (c)	-165.88	-694.04	(1)
C$_3$H$_6$O$_3$	90.0795	DL-Lactic acid (liq)	-160.3	-670.7	(1)
C$_3$H$_6$S	74.1453	Thiacyclobutane (liq)	+5.93	+24.81	(1)
C$_3$H$_7$NO	73.0953	N,N-Dimethylformamide (liq)	-57.2	-239.3	(1)
C$_3$H$_7$NO	73.0953	Propionamide (c)	-81.7	-341.8	(1)
C$_3$H$_7$NO$_2$	89.0947	DL-Alanine (c)	-134.55	-562.96	(1)
C$_3$H$_7$NO$_2$	89.0947	L-Alanine (c)	-133.96	-560.49	(1)
C$_3$H$_7$NO$_2$	89.0947	Ethyl carbamate (c)	-124.4	-520.5	(1)
C$_3$H$_7$NO$_2$	89.0947	Sarcosine (c)	-121.2	-507.1	(1)
C$_3$H$_7$NO$_2$S	121.1587	L-Cysteine (c)	-124.6	-521.3	(1)
C$_3$H$_7$NO$_3$	105.0941	L-Isoserine (c)	-177.8	-743.9	(1)
C$_3$H$_7$NO$_3$	105.0941	L-Serine (c)	-173.6	-726.3	(1)
C$_3$H$_7$N$_5$	113.1227	5-Dimethylaminotetrazole (c)	+43.6	+182.4	(1)
C$_3$H$_7$N$_5$O$_3$	161.1209	1-Acetamido-2-nitroguanidine (c)	-46.3	-193.7	(1)
C$_3$H$_7$N$_5$O$_3$	161.1209	3-Amino-5-methyl-1,2,4-triazole nitrate (c)	-54.6	-228.4	(1)
C$_3$H$_8$	44.0972	Propane (g)	-24.81	-103.81	(1)
C$_3$H$_8$Hg	244.6872	Methyl ethyl mercury (liq)	+11.1	+46.4	(3)
C$_3$H$_8$N$_6$O$_3$	176.1356	1,3-Dimethyl-5-iminotetrazole nitrate (c)	-1.3	-5.4	(1)
C$_3$H$_8$O	60.0966	Methyl ethyl ether (g)	-51.72	-216.40	(1)
C$_3$H$_8$O	60.0966	1-Propanol (liq)	-72.66	-304.01	(1)
C$_3$H$_8$O	60.0966	2-Propanol (liq)	-75.97	-317.96	(1)
C$_3$H$_8$O$_2$	76.0960	1,2-Propanediol (liq)	-119.6	-500.4	(1)
C$_3$H$_8$O$_2$	76.0960	1,3-Propanediol (liq)	-124.4	-520.5	(1)
C$_3$H$_8$O$_3$	92.0954	1,2,3-Propanetriol (liq)	-159.76	-668.44	(1)
C$_3$H$_8$S	76.1612	1-Propanethiol (liq)	-23.78	-99.50	(1)
C$_3$H$_8$S$_2$	108.2252	1,3-Propanedithiol (liq)	-18.83	-73.79	(1)
C$_3$H$_9$Al	72.0867	Trimethyl aluminum (g)	-17.7	-74.1	(2)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	kJ mol⁻¹	Ref
C_3H_9Al	72.0867	Trimethyl aluminum (liq)	-32.6	-136.4	(2)
C_3H_9B	55.9162	Trimethyl boron (g)	-29.7	-124.3	(2)
C_3H_9B	55.9162	Trimethyl boron (liq)	-34.2	-143.1	(2)
$C_3H_9BO_3$	103.9144	Trimethoxyborane (g)	-215.0	-899.6	(2)
$C_3H_9BO_3$	103.9144	Trimethoxyborane (liq)	-223.2	-933.9	(2)
C_3H_9Ga	114.8252	Trimethyl gallium (g)	-10.8	-45.2	(2)
C_3H_9Ga	114.8252	Trimethyl gallium (liq)	-18.7	-79.2	(2)
C_3H_9N	59.1119	Isopropylamine (liq)	-26.83	-112.26	(1)
C_3H_9N	59.1119	n-Propylamine (liq)	-24.26	-101.50	(1)
C_3H_9N	59.1119	Trimethylamine (liq)	-11.0	-46.0	(1)
$C_3H_9N_5O_4$	179.1363	Acetamidoguanidine nitrate (c)	-118.1	-494.1	(1)
C_3H_9P	76.0790	Trimethylphosphine (liq)	-30.	-126.	(1)
$C_3H_{10}N_2$	74.1266	1,2-Propanediamine (liq)	-23.38	-97.82	(1)
$C_3H_{10}N_2O_3$	122.1248	Trimethylamine nitrate (c)	-74.1	-310.0	(1)
$C_3H_{10}O_3Si$	122.1974	Trimethoxysilane (liq)	-199.	-833.	(2)
$C_3H_{10}Sn$	164.8032	Trimethyl tin (g)	+5.	+21.	(2)
$C_3H_{10}Sn$	164.8032	Trimethyl tin (liq)	-2.1	-8.8	(2)
$C_3H_{12}N_6O_3$	180.1675	Guanidine carbonate (c)	-232.10	-971.11	(1)
$C_4H_2N_2S$	110.1379	4-Cyanothiazole (c)	+52.63	+220.20	(1)
$C_4H_2O_3$	98.0587	Maleic anhydride (c)	-112.42	-470.37	(1)
$C_4H_4N_2$	80.0899	Pyrazine (c)	+33.41	+139.79	(1)
$C_4H_4N_2$	80.0899	Pyrazine (g)	+46.86	+196.06	(1)
$C_4H_4N_2$	80.0899	Pyridazine (g)	+66.52	+278.32	(1)
$C_4H_4N_2$	80.0899	Pyridazine (liq)	+53.74	+224.85	(1)
$C_4H_4N_2$	80.0899	Pyrimidine (g)	+46.99	+196.51	(1)
$C_4H_4N_2$	80.0899	Pyrimidine (liq)	+35.04	+146.61	(1)
$C_4H_4N_2O_3$	128.0881	Barbituric acid (c)	-152.2	-636.8	(1)
$C_4H_4N_2O_4$	144.0875	Dialuric acid (c)	-314.4	-1315.4	(1)
$C_4H_4N_2O_5$	160.0869	Alloxan monohydrate (c)	-239.08	-1000.31	(1)
C_4H_4O	68.0759	Furan (g)	-8.23	-34.43	(1)
C_4H_4O	68.0759	Furan (liq)	-14.84	-62.09	(1)
$C_4H_4O_2$	84.0753	β-Methylene-β-propiolactone (liq)	-55.72	-233.13	(1)
$C_4H_4O_3$	100.0747	Succinic anhydride (c)	-143.8	-601.7	(1)
$C_4H_4O_4$	116.0741	Fumaric acid (c)	-193.84	-811.03	(1)
$C_4H_4O_4$	116.0741	Maleic acid (c)	-188.94	-790.52	(1)
C_4H_4S	84.1405	Thiophene (liq)	+19.24	+80.50	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	Formation kJ mol^{-1}	Ref
C_4H_5N	67.0912	Pyrrole (g)	+25.88	+108.28	(1)
C_4H_5N	67.0912	Pyrrole (liq)	+15.08	+63.09	(1)
$C_4H_5NO_3$	115.0894	Sarcosine-N-carboxylic acid anhydride (c)	-144.1	-602.9	(1)
C_4H_5NS	99.1552	4-Methylthiazole (liq)	+16.31	+58.24	(1)
$C_4H_5N_3O_3$	143.1028	Uramil (c)	-168.2	-703.7	(1)
C_4H_6	54.0924	1,2-Butadiene (g)	+38.77	+162.21	(4)
C_4H_6	54.0924	1,3-Butadiene (g)	+26.33	+110.16	(4)
C_4H_6	54.0924	1-Butyne (g)	+39.49	+165.23	(4)
C_4H_6	54.0924	2-Butyne (g)	+34.98	+146.36	(4)
$C_4H_6CuO_6$	213.6288	Copper (II) glycollate (c)	-299.1	-1251.4	(3)
$C_4H_6CuO_4$	181.6300	Copper (II) acetate (c)	-213.5	-893.3	(3)
$C_4H_6MnO_4$	173.0280	Manganese acetate (c)	-274.4	-1148.1	(3)
$C_4H_6N_2O_2$	114.1046	Glycine anhydride (c)	-106.0	-443.5	(1)
$C_4H_6N_2O_2$	114.1046	5-Methyl hydantoin (c)	-115.3	-486.6	(4)
$C_4H_6N_4O_3$	158.1174	Allantoin (c)	-171.51	-717.60	(1)
$C_4H_6N_6$	138.1326	3-Azido-5-ethyl-s-triazole (c)	+87.4	+365.7	(1)
$C_4H_6N_6$	166.1460	1,2-Di-(5-tetrazolyl)ethane (c)	+106.2	+444.3	(1)
$C_4H_6N_{10}$	194.1594	cis-1,1'-Dimethyl-5,5'-azotetrazole (c)	+188.6	+789.1	(1)
$C_4H_6N_{10}$	194.1594	trans-1,1'-Dimethyl-5,5'-azotetrazole (c)			
$C_4H_6N_{10}$	194.1594	2,2'-Dimethyl-5,5'-azotetrazole (c)	+189.3	+792.0	(1)
$C_4H_6O_2$	86.0912	2,3-Butanedione (liq)	+180.3	+754.4	(1)
$C_4H_6O_2$	86.0912	cis-Crotonic acid (liq)	-87.44	-365.85	(1)
$C_4H_6O_2$	86.0912	trans-Crotonic acid (c)	-83.	-347.	(1)
$C_4H_6O_3$	102.0906	Acetic anhydride (liq)	-102.9	-430.5	(1)
$C_4H_6O_4$	118.0900	Dimethyl oxalate (liq)	-149.45	-625.30	(1)
$C_4H_6O_4$	118.0900	Succinic acid (c)	-181.0	-757.3	(1)
$C_4H_6O_4Pb$	325.2800	Lead acetate (c)	-224.79	-940.52	(1)
$C_4H_6O_4Zn$	183.4600	Zinc acetate (c)	-230.36	-963.83	(2)
$C_4H_6O_5$	134.0894	DL-Malic acid (c)	-257.8	-1073.5	(2)
$C_4H_6O_5$	134.0894	L-Malic acid (c)	-264.27	-1105.71	(1)
$C_4H_6O_6$	150.0888	DL-Tartaric acid (c)	-263.78	-1103.66	(1)
$C_4H_6O_6$	150.0888	L-Tartaric acid (c)	-308.5	-1290.8	(1)
$C_4H_6O_6$	150.0888	meso-Tartaric acid (c)	-306.5	-1282.4	(1)
$C_4H_6O_6Zn$	215.4588	Zinc glycollate (c)	-305.9	-1279.9	(1)
			-350.6	-1466.9	(2)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	Enthalpy of Formation kJ mol⁻¹	Ref
C_4H_7NO	85.1065	α-Pyrrolidone (c)	-68.3	-285.8	(1)
$C_4H_7NO_2$	101.1059	Diacetamide (c)	-117.	-490.	(1)
$C_4H_7NO_4$	133.1047	L-Aspartic acid (c)	-232.47	-972.65	(1)
$C_4H_7NO_4$	133.1047	Diglycolamidic acid (c)	-219.5	-918.4	(1)
$C_4H_7N_3O$	113.1199	Creatinine (c)	-56.77	-237.53	(1)
$C_4H_7N_5$	125.1339	1-Allyl-5-aminotetrazole (c)	+63.4	+265.3	(1)
$C_4H_7N_5$	125.1339	2-Allyl-5-aminotetrazole (c)	+67.6	+282.8	(1)
$C_4H_7N_5O_2$	157.1327	5-Tetrazoylurethan (c)	-52.6	-220.1	(1)
$C_4H_7N_7$	153.1473	4-Amino-3-azido-5-ethyl-s-triazole (c)	+118.5	+495.3	(1)
C_4H_8	56.1084	Cyclobutane (liq)	+0.76	+3.19	(4)
C_4H_8	56.1084	1-Butene (g)	-0.03	-0.13	(4)
C_4H_8	56.1084	cis-2-Butene (g)	-1.67	-6.99	(4)
C_4H_8	56.1084	trans-2-Butene (g)	-2.67	-11.17	(4)
C_4H_8	56.1084	2-Methylpropene (g)	-4.04	-16.90	(4)
$C_4H_8N_2O_2$	116.1206	Succinamide (c)	-138.9	-581.2	(1)
$C_4H_8N_2O_3$	132.1200	L-Asparagine (c)	-188.50	-788.68	(1)
$C_4H_8N_2O_3$	132.1200	Glycylglycine (c)	-178.51	-746.89	(1)
$C_4H_8N_2O_4$	148.1194	L-Tartramide (c)	-222.9	-932.6	(1)
$C_4H_8N_2O_4$	148.1194	meso-Tartramide (c)	-223.5	-935.1	(1)
C_4H_8O	72.1078	Butanone (g)	-59.26	-247.94	(1)
C_4H_8O	72.1078	Butanone (liq)	-65.29	-273.17	(1)
C_4H_8O	72.1078	n-Butyraldehyde (liq)	-57.3	-239.7	(1)
C_4H_8O	72.1078	Tetrahydrofuran (g)	-44.03	-184.22	(1)
C_4H_8O	72.1078	Tetrahydrofuran (liq)	-51.1	-213.8	(1)
$C_4H_8O_2$	88.1072	Butyric acid (liq)	-127.59	-533.84	(1)
$C_4H_8O_2$	88.1072	1,3-Dioxane (liq)	-89.99	-376.52	(1)
$C_4H_8O_2$	88.1072	1,4-Dioxane (liq)	-84.47	-353.42	(1)
$C_4H_8O_2$	88.1072	Gycol acetal (liq)	-91.1	-381.2	(1)
$C_4H_8O_3$	104.1066	DL-β-Hydroxybutyric acid (liq)	-162.3	-679.1	(1)
$C_4H_8O_3$	104.1066	Hydroxyisobutyric acid (c)	-177.9	-744.3	(1)
$C_4H_8O_7$	168.1042	DL-Tartaric acid monohydrate (c)	-371.	-1552.	(1)
C_4H_8S	88.1724	Thiacyclopentane (liq)	-17.39	-72.76	(1)
C_4H_9N	71.1230	Pyrrolidine (g)	-0.89	-3.72	(1)
C_4H_9N	71.1230	Pyrrolidine (liq)	-9.87	-41.30	(1)
C_4H_9NO	87.1224	n-Butyramide (c)	-87.5	-366.1	(1)
$C_4H_9NO_2$	103.1218	γ-Aminobutyric acid (c)	-138.1	-577.8	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	Enthalpy of Formation kJ mol⁻¹	Ref
$C_4H_9NO_3$	119.1212	DL-Threonine (c)	-181.4	-759.0	(1)
$C_4H_9NO_3$	119.1212	L-Threonine (c)	-181.4	-759.0	(1)
$C_4H_9N_3O_2$	131.1352	Creatine (c)	-128.16	-536.22	(1)
C_4H_{10}	58.1243	n-Butane (g)	-30.10	-125.94	(1)
$C_4H_{10}Hg$	258.7143	Diethyl mercury (g)	+18.0	+75.3	(3)
$C_4H_{10}Hg$	258.7143	Diethyl mercury (liq)	+7.2	+30.1	(3)
$C_4H_{10}N_2$	86.1377	Piperazine (c)	-10.90	-45.61	(1)
$C_4H_{10}N_2O_4$	150.1353	L-Asparagine monohydrate (c)	-259.52	-1085.83	(1)
$C_4H_{11}N_3O_3$	149.1506	Creatine hydrate (c)	-199.1	-833.0	(1)
$C_4H_{10}O$	74.1237	1-Butanol (liq)	-78.25	-327.40	(1)
$C_4H_{10}O$	74.1237	2-Butanol (liq)	-81.88	-342.59	(1)
$C_4H_{10}O$	74.1237	Diethyl ether (g)	-60.26	-252.13	(1)
$C_4H_{10}O$	74.1237	2-Methyl-1-propanol (liq)	-79.85	-334.09	(1)
$C_4H_{10}O$	74.1237	2-Methyl-2-propanol (liq)	-85.86	-359.24	(1)
$C_4H_{10}O_2$	90.1231	1,2-Dimethoxyethane (liq)	-90.02	-376.64	(1)
$C_4H_{10}O_4$	122.1219	meso-1,2,3,4-Butanetetrol (c)	-217.56	-910.27	(1)
$C_4H_{10}S$	90.1883	1-Butanethiol (liq)	-29.69	-124.22	(1)
$C_4H_{10}S_2$	122.2523	1,4-Butanedithiol (liq)	-25.11	-105.06	(1)
$C_4H_{10}Zn$	123.4943	Diethyl zinc (g)	+12.1	+50.6	(2)
$C_4H_{10}Zn$	123.4943	Diethyl zinc (liq)	+2.5	+10.5	(2)
$C_4H_{11}N$	73.1390	n-Butylamine (liq)	-30.52	-127.70	(1)
$C_4H_{11}N$	73.1390	sec.-Butylamine (liq)	-32.87	-137.53	(1)
$C_4H_{11}N$	73.1390	tert.-Butylamine (liq)	-35.97	-150.50	(1)
$C_4H_{11}N$	73.1390	Diethylamine (liq)	-24.7	-103.3	(1)
$C_4H_{11}N$	73.1390	Isobutylamine (liq)	-31.68	-132.55	(1)
$C_4H_{12}N_2$	88.1536	1,2-Butanediamine (liq)	-28.74	-120.25	(1)
$C_4H_{12}N_2$	88.1536	2-Methyl-1,2-propanediamine (liq)	-32.00	-133.89	(1)
$C_4H_{12}N_2O_3$	136.1518	Diethylamine nitrate (c)	-100.1	-418.8	(2)
$C_4H_{12}O_4Si$	152.2238	Tetramethoxysilane (liq)	-302.	-1264.	(2)
$C_4H_{12}Pb$	267.3302	Tetramethyl lead (g)	+32.48	+135.90	(2)
$C_4H_{12}Pb$	267.3302	Tetramethyl lead (liq)	+23.4	+97.9	(2)
$C_4H_{12}Si$	88.2262	Tetramethylsilane (g)	-57.1	-238.9	(2)
$C_4H_{12}Si$	88.2262	Tetramethylsilane (liq)	-63.	-264.	(2)
$C_4H_{12}Sn$	178.8302	Diethyl tin (g)	+11.0	+46.0	(2)
$C_4H_{12}Sn$	178.8302	Diethyl tin (liq)	+2.1	+8.8	(2)
$C_4H_{12}Sn$	178.8302	Tetramethyl tin (g)	-4.5	-18.8	(2)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	kJ mol⁻¹	Ref
$C_4H_{12}Sn$	178.8302	Tetramethyl tin (liq)	-12.5	-52.3	(2)
$C_4H_{22}N_2O_6$	194.2297	Piperazine hexahydrate (c)	-436.8	-1827.6	(1)
C_4NiO_4	170.7522	Nickel carbonyl (g)	-144.10	-602.91	(3)
C_4NiO_4	170.7522	Nickel carbonyl (liq)	-151.3	-633.0	(3)
C_5FeO_5	195.8998	Iron pentacarbonyl (g)	-175.4	-733.9	(3)
C_5FeO_5	195.8998	Iron pentacarbonyl (liq)	-185.0	-774.0	(3)
$C_5H_4N_4O$	136.1138	Hypoxanthine (c)	-26.24	-109.79	(1)
$C_5H_4N_4O$	136.1138	8-Oxypurine (c)	-15.4	-64.4	(1)
$C_5H_4N_4O_2$	152.1132	Xanthine (c)	-90.49	-379.61	(1)
$C_5H_4N_4O_3$	168.1126	Isouric acid (c)	-147.9	-618.3	(1)
$C_5H_4N_4O_3$	168.1126	Uric acid (c)	-147.73	-618.10	(1)
$C_5H_4O_2$	96.0864	Furfural (liq)	-47.8	-200.0	(1)
$C_5H_4O_3$	112.0858	2-Furoic acid (c)	-119.1	-498.3	(1)
C_5H_5N	79.1023	Pyridine (g)	+33.61	+140.62	(1)
C_5H_5N	79.1023	Pyridine (liq)	+23.96	+100.25	(1)
C_5H_5NO	95.1017	Pyrrolaldehyde (c)	-24.8	-103.8	(1)
$C_5H_5N_5$	135.1291	Adenine (c)	+23.21	+97.11	(1)
$C_5H_5N_5O$	151.1285	Guanine (c)	-43.72	-182.92	(1)
$C_5H_6N_2O$	110.1164	Pyrrolaldoxime	+3.7	+15.5	(1)
$C_5H_6N_2O_2$	126.1158	4-Methyl uracil (c)	-109.2	-456.9	(1)
$C_5H_6N_2O_2$	126.1158	Thymine (c)	-111.9	-468.2	(1)
$C_5H_6N_2O_3$	142.1152	Dimethyl parabanic acid (c)	-137.0	-573.2	(1)
$C_5H_6N_4O_4$	186.1280	Pseudouric acid (c)	-221.7	-927.6	(1)
$C_5H_6O_2$	98.1024	Furfuryl alcohol (liq)	-66.0	-276.1	(1)
$C_5H_6O_2$	98.1024	Levulinic lactone (liq)	-76.2	-318.8	(1)
$C_5H_6O_4$	130.1012	Citraconic acid (c)	-197.04	-824.42	(1)
$C_5H_6O_4$	130.1012	Itaconic acid (c)	-201.06	-841.24	(1)
$C_5H_6O_4$	130.1012	Mesaconic acid (c)	-197.	-824.	(1)
$C_5H_6O_5$	146.1006	α-Ketoglutaric acid (c)	-245.35	-1026.54	(1)
C_5H_6S	98.1676	2-Methyl thiophene (liq)	+10.75	+44.98	(1)
C_5H_6S	98.1676	3-Methyl thiophene (liq)	+10.38	+43.43	(1)
$C_5H_7N_3$	109.1316	2,6-Diaminopyridine (c)	-1.5	-6.3	(1)
C_5H_8	68.1195	2-Methyl-1,3-butadiene (g)	+18.10	+75.73	(4,5)
C_5H_8	68.1195	2-Methyl-1,3-butadiene (liq)	+11.80	+49.37	(4)
C_5H_8	68.1195	1,2-Pentadiene (g)	+33.63	+140.71	(5)
C_5H_8	68.1195	1-cis-3-Pentadiene (g)	+19.79	+82.80	(5)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	Enthalpy of Formation kJ mol^{-1}	Ref
C_5H_8	68.1195	1-trans-3-Pentadiene (g)	+18.13	+75.86	(5)
C_5H_8	68.1195	1,4-Pentadiene (g)	+25.43	+106.40	(5)
C_5H_8	68.1195	2,3-Pentadiene (g)	+31.81	+133.09	(5)
C_5H_8	68.1195	3-Methyl-1-butyne (g)	+32.62	+136.48	(4)
C_5H_8	68.1195	1-Pentyne (g)	+34.52	+144.43	(4)
C_5H_8	68.1195	2-Pentyne (g)	+30.81	+128.91	(4)
C_5H_8	68.1195	Spiropentane (g)	+44.26	+185.18	(5)
$C_5H_8N_2O_2$	128.1317	5,5-Dimethyl hydantoin (c)	-126.4	-528.9	(1)
$C_5H_8N_2O_2$	128.1317	4-Methyl hydrouracil (c)	-125.5	-525.1	(1)
$C_5H_8N_2O_5$	176.1299	Glycylglycine-N-carboxylic acid (c)	-273.0	-1142.2	(1)
$C_5H_8N_4O_3$	172.1445	Methyl allantoin (c)	-177.0	-740.6	(1)
C_5H_8O	84.1189	Dihydropyran, 4H (liq)	-37.5	-156.9	(1)
$C_5H_8O_2$	100.1183	Angelic acid (c)	-108.9	-455.6	(1)
$C_5H_8O_2$	100.1183	Tiglic acid (c)	-117.3	-490.8	(1)
$C_5H_8O_3$	116.1177	Levulinic acid (c)	-166.6	-697.1	(1)
$C_5H_8O_4$	132.1171	Dimethyl malonate (liq)	-190.2	-795.8	(1)
$C_5H_8O_4$	132.1171	Glutaric acid (c)	-229.44	-959.98	(1)
$C_5H_8O_5$	148.1165	D-Arabonic acid-γ-lactone (c)	-238.2	-996.6	(1)
$C_5H_8O_7$	180.1153	DL-Trihydroxyglutaric acid (c)	-356.	-1490.	(1)
C_5H_9N	83.1342	1,2,5,6-Tetrahydropyridine (liq)	+8.0	+33.5	(1)
C_5H_9NO	99.1336	N-Methylpyrrolidone (liq)	-62.64	-262.09	(1)
C_5H_9NO	99.1336	α-Piperidone (c)	-73.3	-306.7	(1)
$C_5H_9NO_2$	115.1330	DL-Proline (c)	-125.7	-525.9	(1)
$C_5H_9NO_3$	131.1324	L-Hydroxyproline (c)	-158.1	-661.5	(1)
$C_5H_9NO_4$	147.1318	L-Glutamic acid (c)	-241.5	-1010.4	(1)
C_5H_{10}	70.1355	Cyclopentane (liq)	-25.28	-105.77	(1)
C_5H_{10}	70.1354	2-Methyl-1-butene (g)	-8.66	-36.23	(4)
C_5H_{10}	70.1354	2-Methyl-2-butene (g)	-10.15	-42.47	(4)
C_5H_{10}	70.1354	3-Methyl-1-butene (g)	-6.90	-28.87	(4)
C_5H_{10}	70.1354	1-Pentene (g)	-4.98	-20.84	(4)
C_5H_{10}	70.1354	cis-2-Pentene (g)	-6.49	-27.15	(4)
C_5H_{10}	70.1354	trans-2-Pentene (g)	-7.57	-31.67	(4)
$C_5H_{10}N_2O_3$	146.1471	DL-Alanylglycine (c)	-185.64	-776.72	(1)
$C_5H_{10}N_2O_3$	146.1471	L-Glutamine (c)	-197.3	-825.5	(1)
$C_5H_{10}O$	86.1349	2-Pentanone (liq)	-71.05	-297.27	(1)
$C_5H_{10}O$	86.1349	3-Pentanone (liq)	-70.87	-296.52	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	Formation kJ mol^{-1}	Ref
$C_5H_{20}O$	86.1349	Tetrahydropyran (g)	-53.39	-223.38	(1)
$C_5H_{10}O$	86.1349	Tetrahydropyran (liq)	-61.1	-255.6	(1)
$C_5H_{10}O$	86.1349	n-Valeraldehyde (liq)	-70.	-293.	(1)
$C_5H_{10}O_2$	102.1343	5-Hydroxy-1-pentanal (liq)	-114.7	-479.9	(1)
$C_5H_{10}O_2$	102.1343	Tetrahydrofurfuryl alcohol (liq)	-104.1	-435.6	(1)
$C_5H_{10}O_2$	102.1343	Valeric acid (liq)	-133.71	-559.44	(1)
$C_5H_{10}O_4$	134.1331	Glyceryl-1-acetate (liq)	-217.5	-910.0	(1)
$C_5H_{10}O_5$	150.1325	β-D-Arabinose (c)	-252.84	-1057.88	(1)
$C_5H_{10}O_5$	150.1325	β-L-Arabinose (c)	-252.84	-1057.88	(1)
$C_5H_{10}O_5$	150.1325	β-D-Ribose (c)	-251.16	-1050.85	(1)
$C_5H_{10}O_5$	150.1325	α-D-Xylose (c)	-252.8	-1057.7	(1)
$C_5H_{10}S$	102.1995	Thiacyclohexane (liq)	-25.33	-105.98	(1)
$C_5H_{11}N$	85.1501	Piperidine (liq)	-21.05	-88.07	(1)
$C_5H_{11}NO_2$	117.1489	6-Aminovaleric acid (c)	-144.5	-604.6	(1)
$C_5H_{11}NO_2$	117.1489	DL-Valine (c)	-148.2	-620.1	(1)
$C_5H_{11}NO_2$	117.1489	L-Valine (c)	-148.2	-620.1	(1)
$C_5H_{11}NO_2S$	149.2129	L-Methionine (c)	-180.4	-754.8	(1)
C_5H_{12}	72.1514	2,2-Dimethylpropane (g)	-39.76	-166.36	(4)
C_5H_{12}	72.1514	2-Methylbutane (g)	-36.91	-154.43	(4)
C_5H_{12}	72.1514	n-Pentane (g)	-35.08	-146.77	(1)
C_5H_{12}	72.1514	n-Pentane (liq)	-41.47	-173.51	(1)
$C_5H_{12}N_2O_2$	132.1636	DL-Ornithine (c)	-156.0	-652.7	(1)
$C_5H_{12}O$	88.1508	1-Pentanol (liq)	-84.27	-352.59	(1)
$C_5H_{12}O_4$	136.1490	Pentaerythritol (c)	-220.0	-920.5	(1)
$C_5H_{12}O_5$	152.1484	L-Arabitol (c)	-268.7	-1124.2	(1)
$C_5H_{12}O_5$	152.1484	Xylitol (c)	-267.32	-1118.47	(1)
$C_5H_{12}S$	104.2154	1-Pentanethiol (liq)	-35.72	-149.45	(1)
C_6CrO_6	220.0593	Chromium hexacarbonyl (g)	-240.4	-1005.8	(3)
C_6CrO_6	220.0593	Chromium hexacarbonyl (c)	-257.4	-1077.0	(3)
$C_6H_4N_2$	104.1122	3-Cyanopyridine (c)	+46.23	+193.43	(1)
$C_6H_5NO_2$	123.1123	Picolinic acid (c)	-83.7	-350.2	(1)
$C_6H_5N_3$	119.1269	Benzotriazole (c)	+59.74	+249.95	(1)
C_6H_6	78.1147	Benzene (g)	+19.81	+82.93	(1)
C_6H_6	78.1147	Benzene (liq)	+11.71	+48.99	(1)
$C_6H_6N_4$	134.1415	7-Methyl purine (c)	+51.3	+214.6	(1)
$C_6H_5N_4O$	150.1409	7-Methylhypoxanthine (c)	-9.9	-41.4	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	kJ mol^{-1}	Ref
C_6H_6O	94.1141	Phenol (c)	-39.45	-165.06	(1)
$C_6H_6O_2$	110.1135	Hydroquinone (c)	-87.47	-365.97	(1)
$C_6H_6O_2$	110.1135	Pyrocatechol (c)	-86.3	-361.1	(1)
$C_6H_6O_2$	110.1135	Resorcinol (c)	-87.95	-367.98	(1)
$C_6H_6O_6$	174.1111	cis-Aconitic acid (c)	-292.7	-1124.7	(1)
$C_6H_6O_6$	174.1111	trans-Aconitic acid (c)	-294.7	-1233.0	(1)
$C_6H_6O_6$	174.1111	D-Mannonic-1,4-3,6-dilactone (c)	-254.6	-1065.2	(1)
C_6H_6S	110.1787	Benzenethiol (liq)	+15.32	+64.10	(1)
C_6H_7N	93.1294	Aniline (liq)	+7.55	+31.59	(1)
C_6H_7N	93.1294	2-Methylpyridine (g)	+24.05	+100.63	(1)
C_6H_7N	93.1294	2-Methylpyridine (liq)	+13.83	+57.85	(1)
C_6H_7N	93.1294	3-Methylpyridine (g)	+26.30	+110.04	(1)
C_6H_7N	93.1294	3-Methylpyridine (liq)	+15.57	+67.14	(1)
C_6H_7N	93.1294	4-Methylpyridine (g)	+24.44	+102.26	(1)
C_6H_7N	93.1294	4-Methylpyridine (liq)	+13.58	+55.82	(1)
$C_6H_8N_2O_3$	156.1423	Aniline nitrate (c)	-43.7	-182.8	(1)
$C_6H_8O_2$	112.1295	Sorbic acid (c)	-93.4	-390.8	(1)
$C_6H_8O_4$	144.1283	Dimethyl fumarate (liq)	-174.3	-729.3	(1)
$C_6H_8O_4$	144.1283	Dimethyl maleate (liq)	-168.2	-703.7	(1)
$C_6H_8O_4$	144.1283	Hexa-2-ene-1,6-dioic acid (c)	-209.	-874.	(1)
$C_6H_8O_4$	144.1283	Hexa-3-ene-1,6-dioic acid (c)	-209.	-874.	(1)
$C_6H_8O_4$	144.1283	Lactide (c)	-184.2	-770.7	(1)
$C_6H_8O_6$	176.1271	L-Ascorbic acid (c)	-278.34	-1164.57	(1)
$C_6H_8O_7$	192.1265	Citric acid, anhydrous (c)	-369.0	-1543.9	(1)
$C_6H_8O_7$	192.1265	D-Glucaric acid-1,4-lactone (c)	-343.2	-1435.9	(1)
$C_6H_8O_7$	192.1265	D-Glucaric acid-3,6-lactone (c)	-343.6	-1437.6	(1)
$C_6H_9AlO_6$	204.1165	Aluminum triacetate (c)	-452.3	-1892.4	(2)
$C_6H_9NO_6$	191.1417	Nitrilotriacetic acid (c)	-312.5	-1307.5	(1)
C_6H_{10}	82.1466	1-Hexyne (g)	+29.57	+123.72	(4)
$C_6H_{10}N_2O_2$	142.1588	Alanine anhydride (c)	-128.0	-535.6	(1)
$C_6H_{10}N_2O_2$	142.1588	5-Methyl-5-ethyl hydantoin (c)	-135.0	-564.8	(1)
$C_6H_{10}N_2O_4$	174.1576	Serine anhydride (c)	-209.5	-876.5	(1)
$C_6H_{10}N_{10}$	222.2136	2,2'-Diethyl-5,5'-azotetrazole (c)	+156.6	+655.2	(1)
$C_6H_{10}O_2$	114.1454	Hydrosorbic acid (liq)	-110.2	-461.1	(1)
$C_6H_{10}O_3$	130.1448	Acetone glyceraldehyde (liq)	-180.	-753.	(1)
$C_6H_{10}O_4$	146.1442	Adipic acid (c)	-237.60	-994.12	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	kJ mol^{-1}	Ref
$C_6H_{10}O_4$	146.1442	Dimethyl succinate (liq)	-199.6	-835.1	(1)
$C_6H_{10}O_4$	146.1442	Erythritol diformal (c)	-161.8	-677.0	(1)
$C_6H_{10}O_4S_2$	210.2722	β,β'-Dithiodilactic acid (liq)	-230.9	-966.1	(1)
$C_6H_{10}O_5$	162.1436	Levoglucosan (c)	-229.3	-959.4	(1)
$C_6H_{10}O_5$	162.1436	Saccharinic acid lactone (c)	-249.6	-1044.3	(1)
$C_6H_{10}O_6$	178.1430	D-Galactonic acid-γ-lactone (c)	-298.3	-1248.1	(1)
$C_6H_{10}O_6$	178.1430	D-Gluconic acid-δ-lactone (c)	-300.3	-1256.5	(1)
$C_6H_{10}O_6$	178.1430	L-Gulonic acid-γ-lactone (c)	-291.5	-1219.6	(1)
$C_6H_{10}O_6$	178.1430	D-Mannonic acid-γ-lactone (c)	-296.2	-1239.3	(1)
$C_6H_{10}O_8$	210.1418	Allomucic acid (c)	-412.	-1724.	(1)
$C_6H_{10}O_8$	210.1418	Citric acid monohydrate (c)	-439.40	-1838.45	(1)
$C_6H_{10}O_8$	210.1418	Mucic acid (c)	-423.	-1770.	(1)
$C_6H_{11}NO$	113.1607	ϵ-Caprolactam (c)	-78.6	-328.9	(1)
$C_6H_{11}NO$	113.1607	N-Methyl piperidone (liq)	-70.00	-292.88	(1)
$C_6H_{11}N_3O_4$	189.1723	Diglycylglycine (c)	-230.8	-965.7	(1)
C_6H_{12}	84.1625	Cyclohexane (liq)	-37.33	-156.19	(1)
C_6H_{12}	84.1625	1-Hexene (g)	-9.94	-41.59	(4)
C_6H_{12}	84.1625	Methylcyclopentane (liq)	-33.06	-138.32	(4)
$C_6H_{12}N_2$	112.1759	Triethylenediamine (c)	-3.4	-14.2	(1)
$C_6H_{12}N_2O_3$	160.1741	Ethyl glycylglycinate (c)	-170.5	-713.4	(1)
$C_6H_{12}N_2O_4S_2$	240.3015	L-Cystine (c)	-245.7	-1028.0	(1)
$C_6H_{12}N_2O_5$	192.1729	Serylserine (c)	-281.8	-1179.1	(1)
$C_6H_{12}N_4$	140.1893	Hexamethylenetetramine (c)	+28.7	+120.1	(1)
$C_6H_{12}N_2S_4$	240.4319	Tetramethylthiuram disulfide (c)	+9.94	+41.59	(1)
$C_6H_{12}N_2S_3$	208.3679	Tetramethylthiuram monosulfide (c)	+11.60	+48.53	(1)
$C_6H_{12}O_2$	116.1613	Caproic acid (liq)	-139.71	-584.55	(1)
$C_6H_{12}O_2$	116.1613	Methyl valerate (liq)	-122.89	-514.17	(1)
$C_6H_{12}O_3$	132.1607	Acetone glycerol (liq)	-163.	-682.	(1)
$C_6H_{12}O_3$	132.1607	Paraldehyde (liq)	-164.2	-687.0	(1)
$C_6H_{12}O_5$	164.1595	D-Fucose (c)	-262.7	-1099.1	(1)
$C_6H_{12}O_5$	164.1595	β-L-Rhamnose (c)	-256.5	-1073.2	(1)
$C_6H_{12}O_6$	180.1589	β-D-Fructose (c)	-302.2	-1264.4	(1)
$C_6H_{12}O_6$	180.1589	α-D-Galactose (c)	-304.1	-1272.4	(1)
$C_6H_{12}O_6$	180.1589	α-D-Glucose (c)	-304.26	-1273.02	(1)
$C_6H_{12}O_6$	180.1589	β-D-Glucose (c)	-302.76	-1266.75	(1)
$C_6H_{12}O_6$	180.1589	D-Mannose (c)	-301.9	-1263.1	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	Formation kJ mol^{-1}	Ref
$C_6H_{12}O_6$	180.1589	L-Sorbose (c)	-303.6	-1270.3	(1)
$C_6H_{12}O_7$	196.1583	D-Galactonic acid (c)	-384.8	-1610.0	(1)
$C_6H_{12}O_7$	196.1583	D-Gluconic acid (c)	-379.3	-1587.0	(1)
$C_6H_{13}NO_2$	131.1760	α-Aminocaproic acid (c)	-152.7	-638.9	(1)
$C_6H_{13}NO_2$	131.1760	γ-Aminocaproic acid (c)	-154.5	-646.4	(1)
$C_6H_{13}NO_2$	131.1760	δ-Aminocaproic acid (c)	-153.7	-643.1	(1)
$C_6H_{13}NO_2$	131.1760	ε-Aminocaproic acid (c)	-152.7	-638.9	(1)
$C_6H_{13}NO_2$	131.1760	DL-Isoleucine (c)	-151.8	-635.1	(1)
$C_6H_{13}NO_2$	131.1760	L-Isoleucine (c)	-151.8	-635.1	(1)
$C_6H_{13}NO_2$	131.1760	D-Leucine (c)	-151.97	-635.84	(1)
$C_6H_{13}NO_2$	131.1760	DL-Leucine (c)	-152.74	-639.06	(1)
$C_6H_{13}NO_2$	131.1760	L-Leucine (c)	-151.97	-635.84	(1)
C_6H_{14}	86.1785	2,2-Dimethylbutane (liq)	-50.99	-213.34	(4)
C_6H_{14}	86.1785	2,3-Dimethylbutane (liq)	-49.46	-206.94	(4)
C_6H_{14}	86.1785	n-Hexane (liq)	-47.50	-198.74	(4)
C_6H_{14}	86.1785	2-Methylpentane (liq)	-48.80	-204.18	(4)
C_6H_{14}	86.1785	3-Methylpentane (liq)	-48.26	-201.92	(4)
$C_6H_{14}N_2O_2$	146.1907	DL-Lysine (c)	-162.2	-678.6	(1)
$C_6H_{14}N_4O_2$	174.2041	L-Arginine (c)	-148.66	-621.99	(1)
$C_6H_{14}N_6O_6$	266.2151	Hexamethylenetetramine dinitrate (c)	-88.6	-370.7	(1)
$C_6H_{14}O$	102.1779	1-Hexanol (liq)	-90.65	-379.28	(1)
$C_6H_{14}O_6$	182.1749	Dulcitol (c)	-321.83	-1346.54	(1)
$C_6H_{14}O_6$	182.1749	D-Mannitol (c)	-319.54	-1336.96	(1)
$C_6H_{14}O_6$	182.1749	α-L-Rhamnose monohydrate (c)	-331.3	-1386.2	(1)
$C_6H_{14}O_7$	198.1743	α-D-Glucose hydrate (c)	-374.97	-1569.87	(1)
$C_6H_{14}S$	118.2425	1-Hexanethiol (liq)	-41.84	-175.06	(1)
$C_6H_{15}B$	97.9974	Triethyl boron (g)	-37.69	-157.69	(2)
$C_6H_{15}B$	97.9974	Triethyl boron (liq)	-46.5	-194.6	(2)
$C_6H_{15}BO_3$	145.9956	Triethoxyborane (g)	-240.4	-1005.8	(2)
$C_6H_{15}BO_3$	145.9956	Triethoxyborane (liq)	-250.8	-1049.3	(2)
$C_6H_{15}N$	101.1932	Triethylamine (liq)	-32.1	-134.3	(1)
$C_6H_{15}O_4P$	182.1578	Triethyl phosphate (liq)	-297.	-1243.	(1)
$C_6H_{16}N_2O_3$	164.2060	Triethylamine nitrate (c)	-98.9	-413.3	(1)
$C_6H_{16}O_3Si$	165.2786	Triethoxysilane (liq)	-226.	-946.	(2)
$C_6H_{16}Si$	116.2804	Triethylsilane (liq)	-54.	-226.	(2)
$C_6H_{18}Al_2$	144.1734	Hexaethyl dialuminum (g)	-55.19	-230.91	(2)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	Formation kJ mol⁻¹	Ref
$C_6H_{18}OSi_2$	162.3818	Hexamethyldisiloxane (g)	-185.88	-777.72	(2)
$C_6H_{18}OSi_2$	162.3818	Hexamethyldisiloxane (liq)	-194.8	-815.0	(2)
$C_6H_{18}Sn_2$	327.5904	Hexamethyl ditin (liq)	-21.6	-90.4	(2)
C_6MoO_6	264.0033	Molybdenum hexacarbonyl (g)	-218.0	-912.1	(3)
C_6MoO_6	264.0033	Molybdenum hexacarbonyl (c)	-234.9	-982.8	(3)
$C_7H_6N_4$	146.1527	1-Phenyltetrazole (c)	+86.5	+361.9	(1)
$C_7H_6N_4$	146.1527	5-Phenyltetrazole (c)	+70.0	+292.9	(1)
$C_7H_6N_4O$	162.1521	1-Phenyl-5-hydroxytetrazole (c)	+26.7	+111.7	(1)
C_7H_6O	106.1253	Benzaldehyde (liq)	-20.1	-84.1	(1)
$C_7H_6O_2$	122.1247	Benzoic acid (c)	-92.03	-385.05	(1)
$C_7H_6O_2$	122.1247	Salicylaldehyde (liq)	-66.9	-279.9	(1)
$C_7H_6O_3$	138.1241	Salicylic acid	-140.9	-589.5	(1)
C_7H_7N	105.1405	2-Vinylpyridine (liq)	+37.2	+155.6	(1)
C_7H_7NO	121.1399	Benzamide (c)	-48.42	-202.59	(1)
C_7H_7NO	121.1399	Formanilide (c)	-36.2	-151.5	(1)
$C_7H_7NO_2$	137.1393	m-Aminobenzoic acid (c)	-98.2	-410.9	(1)
$C_7H_7NO_2$	137.1393	o-Aminobenzoic acid (c)	-95.8	-400.8	(1)
$C_7H_7NO_2$	137.1393	p-Aminobenzoic acid (c)	-98.8	-413.4	(1)
$C_7H_7N_5$	161.1673	1-Phenyl-5-aminotetrazole (c)	+74.3	+310.9	(1)
$C_7H_7N_5$	161.1673	5-Phenylaminotetrazole (c)	+72.9	+305.0	(1)
C_7H_8	92.1418	Toluene (liq)	+2.88	+12.05	(4)
$C_7H_8N_4O_2$	180.1674	Theobromine (c)	-86.4	-361.5	(1)
C_7H_8O	108.1412	m-Cresol (c)	-46.37	-194.01	(1)
C_7H_8O	108.1412	o-Cresol (c)	-48.90	-204.60	(1)
C_7H_8O	108.1412	p-Cresol (c)	-47.63	-199.28	(1)
C_7H_8S	124.2058	Benzyl mercaptan (liq)	+10.5	+43.9	(1)
C_7H_8S	124.2058	Phenylmethylsulfide (liq)	+11.5	+48.1	(1)
C_7H_9N	107.1565	2,3-Dimethylpyridine (liq)	+4.62	+19.33	(1)
C_7H_9N	107.1565	2,4-Dimethylpyridine (liq)	+3.85	+16.11	(1)
C_7H_9N	107.1565	2,5-Dimethylpyridine (liq)	+4.45	+18.62	(1)
C_7H_9N	107.1565	2,6-Dimethylpyridine (liq)	+3.02	+12.64	(1)
C_7H_9N	107.1565	3,4-Dimethylpyridine (liq)	+4.36	+18.24	(1)
C_7H_9N	107.1565	3,5-Dimethylpyridine (liq)	+5.36	+22.43	(1)
C_7H_9N	107.1565	2-Ethylpyridine (liq)	-1.2	-5.0	(1)
C_7H_9N	107.1565	N-Methylaniline (liq)	+7.7	+32.2	(1)
$C_7H_{10}O_4$	158.1554	Terebic acid (c)	-222.	-929.	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	Enthalpy of Formation kJ mol^{-1}	Ref
$C_7H_{10}O_4$	158.1554	Tetraconic acid (c)	-204.	-954.	(1)
$C_7H_{11}N_5$	165.1992	1-Allyl-5-allylaminotetrazole (c)	+83.7	+350.2	(1)
$C_7H_{11}N_5$	165.1992	5-Diallylaminotetrazole (c)	+83.9	+351.0	(1)
C_7H_{12}	96.1737	1-Heptyne (g)	+24.64	+103.09	(4)
$C_7H_{12}N_2O_2$	156.1859	Glycylvalyl anhydride (c)	-120.5	-504.2	(1)
$C_7H_{12}O_4$	160.1713	Dimethyl glutarate (liq)	-205.9	-861.5	(1)
$C_7H_{12}O_5$	176.1707	Glyceryl-1,3-diacetate (liq)	-268.2	-1122.1	(1)
$C_7H_{12}O_7$	208.1695	D-Gluco-D-guloheptonic acid-γ-lactone (c)	-355.6	-1497.8	(1)
$C_7H_{13}NO$	127.1878	5-Enantholactam (c)	-83.2	-348.1	(1)
$C_7H_{13}NO$	127.1878	N-Methylcaprolactam (liq)	-73.3	-306.7	(1)
$C_7H_{13}NO$	127.1878	5-Methylcaprolactam (c)	-86.9	-353.6	(1)
$C_7H_{13}NO$	127.1878	7-Methylcaprolactam (c)	-86.5	-361.9	(1)
$C_7H_{13}NO_3$	159.1866	N-Formyl-DL-leucine (c)	-222.1	-929.3	(1)
C_7H_{14}	98.1896	Cycloheptane (liq)	-37.47	-156.77	(1)
C_7H_{14}	98.1896	1-Heptene (g)	-14.87	-62.22	(4)
C_7H_{14}	98.1896	1,1-Dimethylcyclopentane (liq)	-41.12	-172.05	(4)
C_7H_{14}	98.1896	cis-1,2-Dimethylcyclopentane (liq)	-39.50	-165.27	(4)
C_7H_{14}	98.1896	trans-1,2-Dimethylcyclopentane (liq)	-40.92	-171.21	(4)
C_7H_{14}	98.1896	cis-1,3-Dimethylcyclopentane (liq)	40.17	-168.07	(4)
C_7H_{14}	98.1896	trans-1,3-Dimethylcyclopentane (liq)	-40.66	-170.12	(4)
C_7H_{14}	98.1896	Ethylcyclopentane (liq)	-39.06	-163.43	(4)
C_7H_{14}	98.1896	Methylcyclohexane (liq)	-45.43	-190.08	(4)
$C_7H_{14}N_2O_3$	174.2012	Glycylvaline (c)	-200.0	-836.8	(1)
$C_7H_{14}O_2$	114.1890	n-Heptaldehyde (liq)	-74.4	-311.3	(1)
$C_7H_{14}O_2$	130.1884	Enanthic acid (liq)	-145.75	-609.82	(1)
$C_7H_{14}O_2$	130.1884	Methyl caproate (liq)	-129.10	-540.15	(1)
$C_7H_{14}O_6$	194.1860	β-Methyl-D-glucofuranoside (liq)	-287.5	-1202.9	(1)
$C_7H_{14}O_6$	194.1860	α-Methyl-D-glucopyranoside (c)	-294.8	-1233.4	(1)
$C_7H_{14}O_6$	194.1860	β-Methyl-D-glucopyranoside (c)	-295.8	-1237.6	(1)
$C_7H_{14}O_7$	210.1854	D-Gluco-α-heptose (c)	-353.5	-1479.0	(1)
$C_7H_{15}NO_2$	145.2031	5-Aminoenanthylic acid (c)	-159.6	-667.8	(1)
C_7H_{16}	100.2056	2,2-Dimethylpentane (liq)	-57.03	-238.61	(4)
C_7H_{16}	100.2056	2,3-Dimethylpentane (liq)	-55.79	-233.43	(1)
C_7H_{16}	100.2056	2,4-Dimethylpentane (liq)	-56.15	-234.93	(4)
C_7H_{16}	100.2056	3,3-Dimethylpentane (liq)	-56.05	-234.51	(4)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	Enthalpy of Formation kJ mol^{-1}	Ref
C_7H_{16}	100.2056	3-Ethylpentane (liq)	-53.75	-224.89	(4)
C_7H_{16}	100.2056	n-Heptane (liq)	-53.61	-224.30	(4)
C_7H_{16}	100.2056	2-Methylhexane (liq)	-54.91	-229.74	(4)
C_7H_{16}	100.2056	3-Methylhexane (liq)	-54.33	-227.32	(4)
C_7H_{16}	100.2056	2,2,3-Trimethylbutane (liq)	-56.61	-236.86	(4)
$C_7H_{16}O_7$	212.2014	D-Gluco-α-heptite (c)	-364.5	-1525.1	(1)
$C_7H_{16}O_7$	212.2014	D-Perseitol (c)	-369.7	-1546.8	(1)
$C_8H_5NO_2$	147.1346	Isatin (c)	-62.7	-262.3	(1)
$C_8H_6N_4O_6$	254.1602	Hydurilic acid (c)	-299.2	-1251.9	(1)
$C_8H_6N_6$	186.1772	3-Azido-5-phenyl-s-triazole (c)	+127.1	+531.8	(1)
$C_8H_6O_3$	150.1352	Phenylglyoxylic acid (c)	-115.3	-482.4	(1)
$C_8H_6O_4$	166.1346	m-Phthalic acid (c)	-191.91	-802.95	(1)
$C_8H_6O_4$	166.1346	o-Phthalic acid (c)	-186.91	-732.03	(1)
$C_8H_6O_4$	166.1346	p-Phthalic acid (c)	-195.05	-816.09	(1)
C_8H_7N	117.517	Indole (c)	+29.8	+124.7	(1)
C_8H_7NO	133.1511	Oxindole (c)	-41.2	-172.4	(1)
$C_8H_7NO_2$	149.1505	Dioxindole (c)	-76.9	-321.7	(1)
$C_8H_7N_7$	201.1919	4-Amino-3-azido-5-phenyl-s-triazole (c)	+159.5	+667.3	(1)
C_8H_8	104.1530	Ethenylbenzene (liq)	+24.84	+103.93	(4)
$C_8H_8N_2O_2$	164.1652	Phthalamide (c)	-104.4	-436.8	(1)
$C_8H_8N_4$	160.1798	1-Methyl-5-phenyltetrazole (c)	+69.9	+292.5	(1)
$C_8H_8N_4$	160.1798	1-Phenyl-5-methyltetrazole (c)	+69.9	+292.5	(1)
$C_8H_8N_4$	160.1798	2-Phenyl-5-methyltetrazole (c)	+65.7	+274.9	(1)
$C_8H_8N_6O_6$	284.1896	Murexide (c)	-289.7	-1212.1	(1)
C_8H_8O	120.1524	Acetophenone (liq)	-34.07	-142.55	(1)
$C_8H_8O_2$	136.1518	Methyl benzoate (liq)	-79.8	-333.9	(1)
$C_8H_8O_2$	136.1518	Phenylacetic acid (c)	-95.3	-398.7	(1)
$C_8H_8O_3$	152.1512	DL-Mandelic acid (c)	-138.5	-579.5	(1)
$C_8H_8O_3$	152.1512	L-Mandelic acid (c)	-138.8	-580.7	(1)
$C_8H_8O_3$	152.1512	Methyl salicylate (liq)	-127.1	-531.9	(1)
$C_8H_8O_3$	152.1512	Phenoxyacetic acid (c)	-122.8	-513.8	(1)
C_8H_9NO	135.1670	Acetanilide (c)	-50.3	-210.5	(1)
$C_8H_9NO_2$	151.1664	α-Phenyl glycine (c)	-103.2	-431.8	(1)
$C_8H_9NO_2$	151.1664	N-Phenyl glycine (c)	-96.2	-402.5	(1)
C_8H_{10}	106.1689	Ethylbenzene (liq)	-2.95	-12.34	(4)
C_8H_{10}	106.1689	m-Xylene (liq)	-6.06	-25.36	(4)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	Enthalpy of Formation kJ mol^{-1}	Ref
C_8H_{10}	106.1689	o-Xylene (liq)	-5.82	-24.35	(4)
C_8H_{10}	106.1689	p-Xylene (liq)	-5.82	-24.35	(4)
$C_8H_{10}N_4O_2$	194.1945	Caffeine (c)	-76.2	-318.8	(1)
$C_8H_{10}N_4O_{10}$	322.1897	Alloxantin dihydrate (c)	-510.3	-2135.1	(1)
$C_8H_{10}O$	122.1683	2-Ethylphenol (c)	-49.91	-208.82	(1)
$C_8H_{10}O$	122.1683	3-Ethylphenol (c)	-51.21	-214.26	(1)
$C_8H_{10}O$	122.1683	4-Ethylphenol (c)	-53.63	-244.39	(1)
$C_8H_{11}N$	121.1836	N,N-Dimethylaniline (liq)	+8.2	+34.3	(1)
$C_8H_{12}N_2O_3$	184.1964	Diethylbarbituric acid (c)	-178.7	-747.7	(1)
$C_8H_{12}Pb$	315.3748	Tetravinyl lead (liq)	+213.	+891.	(2)
$C_8H_{12}Sn$	226.8748	Tetravinyl tin (liq)	+72.	+301.	(2)
C_8H_{14}	110.2008	1-Octyne (g)	+19.73	+82.55	(4)
$C_8H_{14}N_2O_2$	170.2130	Valylalanyl anhydride (c)	-123.3	-515.9	(1)
$C_8H_{14}N_4O_5$	246.2246	Triglycylglycine (c)	-284.7	-1191.2	(1)
$C_8H_{14}O_4$	174.1984	Dimethyl adipate (liq)	-211.9	-886.6	(1)
$C_8H_{14}O_4$	174.1984	Erythritol diacetal (c)	-182.	-761.	(1)
$C_8H_{14}O_8$	238.1960	D-Gluco-α,α-octonic acid-γ-lactone (c)	-394.2	-1649.3	(1)
C_8H_{16}	112.2167	Cyclooctane (liq)	-40.58	-169.79	(1)
C_8H_{16}	112.2167	1-Octene (g)	-19.80	-82.84	(4)
C_8H_{16}	112.2167	1,1-Dimethylcyclohexane (liq)	-52.28	-218.74	(4)
C_8H_{16}	112.2167	cis-1,2-Dimethylcyclohexane (liq)	-50.62	-211.79	(4)
C_8H_{16}	112.2167	trans-1,2-Dimethylcyclohexane (liq)	-52.16	-218.24	(4)
C_8H_{16}	112.2167	cis-1,3-Dimethylcyclohexane (liq)	-53.27	-222.88	(4)
C_8H_{16}	112.2167	trans-1,3-Dimethylcyclohexane (liq)	-51.55	-215.69	(4)
C_8H_{16}	112.2167	cis-1,4-Dimethylcyclohexane (liq)	-51.53	-215.60	(4)
C_8H_{16}	112.2167	trans-1,4-Dimethylcyclohexane (liq)	-53.15	-222.38	(4)
C_8H_{16}	112.2167	Ethylcyclohexane (liq)	-50.70	-212.13	(4)
C_8H_{16}	112.2167	n-Propylcyclopentane (liq)	-45.19	-189.07	(4)
$C_8H_{16}N_2O_3$	188.2283	DL-Leucylglycine (c)	-205.07	-853.01	(1)
$C_8H_{16}O$	128.2161	n-Octaldehyde (liq)	-80.0	-334.7	(1)
$C_8H_{16}O_2$	144.2155	Caprylic acid (liq)	-151.93	-635.68	(1)
$C_8H_{16}O_2$	144.2155	Methyl enanthate (liq)	-135.53	-567.06	(1)
$C_8H_{17}N$	127.2314	Coniine (liq)	-57.6	-241.0	(1)
C_8H_{18}	114.2327	2,2-Dimethylhexane (liq)	-62.60	-251.92	(4)
C_8H_{18}	114.2327	2,3-Dimethylhexane (liq)	-60.38	-252.63	(4)
C_8H_{18}	114.2327	2,4-Dimethylhexane (liq)	-61.44	-257.06	(4)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	Formation kJ mol⁻¹	Ref
C_8H_{18}	114.2327	2,5-Dimethylhexane (liq)	-62.24	-260.41	(4)
C_8H_{18}	114.2327	3,3-Dimethylhexane (liq)	-61.56	-257.57	(4)
C_8H_{18}	114.2327	3,4-Dimethylhexane (liq)	-60.20	-251.88	(4)
C_8H_{18}	114.2327	3-Ethylhexane (liq)	-59.85	-250.41	(4)
C_8H_{18}	114.2327	2-Methyl-3-ethylpentane (liq)	-59.66	-249.62	(4)
C_8H_{18}	114.2327	3-Methyl-3-ethylpentane (liq)	-60.44	-252.88	(4)
C_8H_{18}	114.2327	2-Methylheptane (liq)	-60.96	-255.06	(4)
C_8H_{18}	114.2327	3-Methylheptane (liq)	-60.32	-252.38	(4)
C_8H_{18}	114.2327	4-Methylheptane (liq)	-60.15	-251.67	(4)
C_8H_{18}	114.2327	n-Octane (liq)	-59.71	-249.83	(4)
C_8H_{18}	114.2327	2,2,3,3-Tetramethylbutane (c)	-64.21	-268.65	(4)
C_8H_{18}	114.2327	2,2,3-Trimethylpentane (liq)	-61.41	-256.94	(4)
C_8H_{18}	114.2327	2,2,4-Trimethylpentane (liq)	-61.95	-259.20	(4)
C_8H_{18}	114.2327	2,3,3-Trimethylpentane (liq)	-60.60	-253.55	(4)
C_8H_{18}	114.2327	2,3,4-Trimethylpentane (liq)	-60.96	-255.06	(4)
$C_8H_{20}Ge$	188.8386	Tetraethyl germanium (liq)	-49.5	-207.1	(2)
$C_8H_{20}Pb$	323.4386	Tetraethyl lead (g)	+26.19	+109.58	(2)
$C_8H_{20}Pb$	323.4386	Tetraethyl lead (liq)	+12.6	+52.7	(2)
$C_8H_{20}O_4Si$	208.3322	Tetraethoxysilane (liq)	-334.	-1397.	(1)
$C_8H_{20}Si$	144.3346	Tetraethylsilane (liq)	-68.	-285.	(2)
$C_8H_{20}Sn$	234.9386	Tetraethyl tin (g)	-10.9	-45.6	(2)
$C_8H_{20}Sn$	234.9386	Tetraethyl tin (liq)	-22.9	-95.8	(2)
C_9H_7N	129.1628	Isoquinoline (c)	+37.9	+158.6	(1)
C_9H_7N	129.1628	Quinoline (liq)	+37.3	+156.1	(1)
C_9H_7NO	145.1622	8-Hydroxyquinoline (c)	-19.9	-83.3	(1)
$C_9H_8N_2O$	160.1769	Dl-α-pyrrylketone (c)	-4.7	-19.7	(1)
C_9H_9N	131.1788	α-Methylindole (c)	+14.5	+60.7	(1)
C_9H_9N	131.1788	Skatole (c)	+16.3	+68.2	(1)
$C_9H_9NO_3$	179.1770	Hippuric acid (c)	-145.63	-609.32	(1)
$C_9H_{10}O_4$	182.1777	DL-Phenylglyceric acid (c)	-178.5	-746.8	(1)
$C_9H_{10}N_2$	146.1934	Dipyrrylmethane (c)	+31.4	+131.4	(1)
$C_9H_{11}NO_2$	165.1935	DL-Phenylalanine (c)	-111.9	-468.2	(1)
$C_9H_{11}NO_2$	165.1935	L-Phenylalanine (c)	-111.9	-468.2	(1)
$C_9H_{11}NO_3$	181.1929	L-Tyrosine (c)	-163.4	-683.7	(1)
C_9H_{12}	120.1960	Isopropylbenzene (liq)	-9.83	-41.13	(4)
C_9H_{12}	120.1960	1-Methyl-2-ethylbenzene (liq)	-11.09	-46.40	(4)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	Formation kJ mol⁻¹	Ref
C_9H_{12}	120.1960	1-Methyl-3-ethylbenzene (liq)	-11.64	-48.70	(4)
C_9H_{12}	120.1960	1-Methyl-4-ethylbenzene (liq)	-11.90	-49.79	(4)
C_9H_{12}	120.1960	n-Propylbenzene (liq)	-9.16	-38.33	(4)
C_9H_{12}	120.1960	1,2,3-Trimethylbenzene (liq)	-13.99	-58.53	(4)
C_9H_{12}	120.1960	1,2,4-Trimethylbenzene (liq)	-14.77	-61.80	(4)
C_9H_{12}	120.1960	1,3,5-Trimethylbenzene (liq)	-15.16	-63.43	(4)
$C_9H_{14}O_6$	218.2083	Glyceryl triacetate (liq)	-318.3	-1331.8	(1)
$C_9H_{14}O_6$	218.2083	Mannitol triformal (c)	-242.	-1013.	(1)
$C_9H_{15}N$	137.2266	Phyllopyrrole (c)	-20.4	-85.4	(1)
C_9H_{16}	124.2279	1-Nonyne (g)	+14.80	+61.92	(4)
$C_9H_{16}N_2O_5$	232.2383	α-Carbethoxyglycylglycine ethyl ester (c)	-275.3	-1151.9	(1)
$C_9H_{16}N_2O_5$	232.2383	β-Carbethoxyglycylglycine ethyl ester (c)	-303.5	-1259.8	(1)
C_9H_{18}	126.2438	1-Nonene (g)	-24.71	-103.39	(4)
C_9H_{18}	126.2438	n-Propylcyclohexane (liq)	-56.95	-238.28	(4)
$C_9H_{18}O_2$	158.2426	Methyl caprylate (liq)	-141.07	-590.24	(1)
$C_9H_{18}O_2$	158.2426	Pelargonic acid (liq)	-157.67	-659.69	(1)
$C_9H_{19}NO_2$	173.2573	ω-Aminopelargonic acid (c)	-174.1	-728.4	(1)
C_9H_{20}	128.2598	n-Nonane (liq)	-65.81	-275.35	(4)
$C_9H_{21}N$	143.2744	Tri-n-propylamine (liq)	-49.51	-207.15	(1)
$C_9H_{21}O_4P$	224.2391	Tri-n-propyl phosphate (liq)	-315.	-1318.	(1)
$C_{10}H_8$	128.1753	Naphthalene (c)	+18.0	+75.3	(1)
$C_{10}H_8$	128.1753	Naphthalene (g)	+35.6	+149.0	(1)
$C_{10}H_8N_2O_2$	188.1875	4-Phenyluracil (c)	-81.7	-341.8	(1)
$C_{10}H_9N$	143.1899	α-Phenylpyrrole (c)	+34.5	+144.3	(1)
$C_{10}H_9N$	143.1899	N-Phenylpyrrole (c)	+38.1	+159.4	(1)
$C_{10}H_9N$	143.1899	Quinaldine (c)	+39.3	+164.4	(1)
$C_{10}H_9NO_3$	191.1881	Phenylalanine-N-carboxylic acid anhydride (c)	-132.3	-553.5	(1)
$C_{10}H_{10}O_4$	194.1888	Dimethyl m-phthalate (c)	-171.	-715.	(1)
$C_{10}H_{10}O_4$	194.1888	Dimethyl o-phthalate (liq)	-162.	-678.	(1)
$C_{10}H_{10}O_4$	194.1888	Dimethyl p-phthalate (c)	-170.	-711.	(1)
$C_{10}H_{11}NO_3$	193.2041	DL-Benzoylalanine (c)	-147.9	-618.8	(1)
$C_{10}H_{11}NO_3$	193.2041	Benzoyl sarcosine (c)	-135.7	-567.8	(1)
$C_{10}H_{11}NO_3$	193.2041	Phenaceturic acid (c)	-151.0	-631.8	(1)
$C_{10}H_{11}NO_3$	193.2041	m-Toluyl glycine (c)	-148.8	-622.6	(1)
$C_{10}H_{11}NO_3$	193.2041	o-Toluyl glycine (c)	-148.3	-620.5	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	Enthalpy of Formation kJ mol⁻¹	Ref
$C_{10}H_{11}NO_3$	193.2041	p-Toluyl glycine (c)	-148.5	-621.3	(1)
$C_{10}H_{11}NO_4$	209.2035	Anisoyl glycine (c)	-180.9	-756.9	(1)
$C_{10}H_{12}O_4$	196.2047	Glyceryl-1-benzoate (c)	-185.80	-777.39	(1)
$C_{10}H_{12}O_4$	196.2047	Glyceryl-2-benzoate (c)	-184.71	-772.83	(1)
$C_{10}H_{13}NO_2$	179.2206	Phenacetin (c)	-101.1	-423.0	(1)
$C_{10}H_{14}N_2$	162.2365	Nicotine (liq)	+9.4	+39.3	(1)
$C_{10}H_{16}N_2O_8$	292.2476	Ethylenediaminetetraacetic acid (c)	-420.5	-1759.4	(1)
$C_{10}H_{16}O_2$	168.2378	Dehydro-β-campholenolactone (c) (dextrorotatory)	-130.	-554.	(1)
$C_{10}H_{16}O_2$	168.2378	Dehydro-β-campholenolactone (c) (inactive)	-137.	-573.	(1)
$C_{10}H_{16}O_3$	184.2372	Methyl ethyl heptane lactone (c) (racemic)	-183.5	-767.8	(1)
$C_{10}H_{18}$	138.2550	1-Decyne (g)	+9.88	+41.34	(4)
$C_{10}H_{19}N_3O_4$	245.2806	Leucylglycylglycine (c)	-259.6	-1086.2	(1)
$C_{10}H_{20}$	140.2709	1-Decene (g)	-29.64	-124.01	(4)
$C_{10}H_{20}O_2$	172.2697	Capric acid (c)	-170.59	-713.75	(1)
$C_{10}H_{20}O_2$	172.2697	Capric acid (liq)	-163.6	-684.5	(1)
$C_{10}H_{20}O_2$	172.2697	Methyl pelargonate (liq)	-147.29	-616.26	(1)
$C_{10}H_{22}$	142.2868	n-Decane (liq)	-71.92	-300.91	(4)
$C_{10}H_{22}O_2$	174.2856	1,10-Decanediol (c)	-165.78	-693.62	(1)
$C_{10}H_{22}O_7$	254.2826	Dipentaerythritol (c)	-376.9	-1576.9	(1)
$C_{11}H_{12}N_2O_2$	204.2305	Glycylphenylalanyl anhydride (c)	-82.9	-346.9	(1)
$C_{11}H_{12}N_2O_2$	204.2305	L-Tryptophan (c)	-99.8	-417.6	(1)
$C_{11}H_{12}N_2O_3$	220.2299	Glycyltyrosyl anhydride (c)	-122.8	-513.8	(1)
$C_{11}H_{12}N_2O_4$	236.2293	Hippurylglycine (c)	-198.54	-830.69	(1)
$C_{11}H_{13}NO_3$	207.2312	o-Toluyl alanine (c)	-156.5	-654.8	(1)
$C_{11}H_{13}NO_3$	207.2312	p-Toluyl alanine (c)	-159.0	-665.3	(1)
$C_{11}H_{14}N_2O_3$	222.2458	Glycylphenylalanine (c)	-163.9	-685.8	(1)
$C_{11}H_{20}$	152.2820	1-Undecyne (g)	+4.96	+20.75	(4)
$C_{11}H_{20}N_2O_2$	212.2943	Valylleucyl anhydride (c)	-150.1	-628.0	(1)
$C_{11}H_{20}O_2$	184.2809	Undecyl-10-ene-1-oic acid (c)	-138.	-577.	(1)
$C_{11}H_{22}$	154.2980	1-Undecene (g)	-34.57	-144.64	(4)
$C_{11}H_{22}O_2$	186.2968	Methyl caprate (liq)	-153.07	-640.44	(1)
$C_{11}H_{24}$	156.3139	n-Undecane (liq)	-78.02	-325.44	(4)
$C_{12}H_8N_2$	180.2110	Phenazine (c)	+56.4	+236.0	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	kJ mol⁻¹	Ref
$C_{12}H_9N$	167.2122	Carbazole (c)	+30.3	+126.9	(1)
$C_{12}H_{10}S$	186.2775	Diphenyl sulfide (c)	+39.1	+163.6	(1)
$C_{12}H_{10}S_2$	218.3415	Diphenyl disulfide (c)	+35.8	+149.8	(1)
$C_{12}H_{14}N_2O_2$	218.2576	Alanylphenylalanyl anhydride (c)	-89.3	-373.6	(1)
$C_{12}H_{14}N_4O_6$	310.2686	Desoxyawamalic acid (c)	-285.7	-1195.4	(1)
$C_{12}H_{14}N_4O_8$	342.2674	Amalic acid (c)	-367.0	-1535.5	(1)
$C_{12}H_{15}NO_4$	237.2577	DL-Phenylalanine-N-carboxylic acid dimethyl ester (c)	-184.3	-771.1	(1)
$C_{12}H_{16}N_2O_3$	236.2729	Alanylphenylalanine (c)	-170.2	-712.1	(1)
$C_{12}H_{16}O_8$	288.2565	Levoglucosan triacetate (c)	-371.3	-1553.5	(1)
$C_{12}H_{18}O_2$	197.2761	3(a)-Hydroxy-trans-decalin-2(a)-acetic acid lactone (c) (boat form)	-133.09	-556.85	(1)
$C_{12}H_{18}O_2$	194.2761	3(e)-Hydroxy-trans-decalin-2(e)-acetic acid lactone (c) (chair form)	-137.26	-574.30	(1)
$C_{12}H_{18}O_8$	290.2725	1,2-Anhydroglucose-3,5,6-triacetate (c)	-411.7	-1722.6	(1)
$C_{12}H_{18}O_8$	260.2896	Mannitol triacetal (c)	-275.	-1151.	(1)
$C_{12}H_{22}$	166.3091	1-Dodecyne (g)	+0.03	+0.13	(4)
$C_{12}H_{22}N_2O_2$	226.3213	Leucine anhydride (c)	-160.0	-669.4	(1)
$C_{12}H_{22}O_6$	262.3055	1,2,5,6-Diacetonemannitol (c)	-350.	-1464.	(1)
$C_{12}H_{22}O_{11}$	342.3025	Cellobiose (c)	-532.5	-2228.0	(1)
$C_{12}H_{22}O_{11}$	342.3025	β-Lactose (c)	-530.1	-2217.9	(1)
$C_{12}H_{22}O_{11}$	342.3025	Maltose (c)	-530.8	-2220.9	(1)
$C_{12}H_{22}O_{11}$	342.3025	Sucrose (c)	-531.9	-2225.5	(1)
$C_{12}H_{22}O_{11}$	342.3025	Trehalose (c)	-531.3	-2223.0	(1)
$C_{12}H_{24}$	168.3251	1-Dodecene (g)	-39.48	-165.18	(4)
$C_{12}H_{24}O_2$	200.3239	Lauric acid (c)	-185.14	-774.63	(1)
$C_{12}H_{24}O_2$	200.3239	Lauric acid (liq)	-176.4	-738.1	(1)
$C_{12}H_{24}O_2$	200.3239	Methyl undecylate (liq)	-158.97	-665.13	(1)
$C_{12}H_{24}O_{12}$	360.3179	α-Lactose monohydrate (c)	-602.	-2519.	(1)
$C_{12}H_{24}O_{12}$	360.3179	β-Maltose monohydrate (c)	-606.	-2536.	(1)
$C_{12}H_{26}$	170.3410	n-Dodecane (liq)	-84.12	-351.96	(4)
$C_{12}H_{26}N_2O_4$	262.3520	Hexamethylene-1,6-diamine-adipic acid Adduct (c)	-305.5	-1278.2	(1)
$C_{12}H_{26}O_{13}$	378.3332	Trehalose dihydrate (c)	-676.1	-2828.3	(1)
$C_{12}H_{27}OP$	218.3222	Tri-n-butyl phosphine oxide (c)	-110.	-460.	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	Enthalpy of Formation kJ mol⁻¹	Ref
$C_{12}H_{27}O_2P$	234.3216	n-Butyl ester of di-n-butyl phosphinic acid (liq)	-183.	-766.	(1)
$C_{12}H_{27}O_4P$	266.3204	Triisobutyl phosphate (liq)	-346.	-1448.	(1)
$C_{12}H_{27}O_4P$	266.3204	Tri-n-butyl phosphate (liq)	-348.	-1456.	(1)
$C_{13}H_9N$	179.2234	Acridine (c)	+44.8	+187.4	(1)
$C_{13}H_{10}O$	182.2241	Benzophenone (c)	-8.0	-33.5	(1)
$C_{13}H_{11}NO$	197.2387	Benzanilide (c)	-22.3	-93.3	(1)
$C_{13}H_{24}$	180.3362	1-Tridecyne (g)	-4.89	-20.46	(4)
$C_{13}H_{26}$	182.3522	1-Tridecene (g)	-44.41	-185.81	(4)
$C_{13}H_{26}O_2$	214.3510	Methyl laurate (liq)	-165.66	-693.12	(1)
$C_{13}H_{26}O_4$	246.3498	Glyceryl-1-caprate (c)	-265.05	-1108.97	(1)
$C_{13}H_{26}O_4$	246.3498	Glyceryl-2-caprate (c)	-261.90	-1095.79	(1)
$C_{13}H_{28}$	184.3681	n-Tridecane (liq)	-90.22	-377.48	(4)
$C_{14}H_{10}$	178.2358	Anthracene (c)	+29.0	+121.3	(1)
$C_{14}H_{10}$	178.2358	Anthracene (g)	+53.7	+224.7	(1)
$C_{14}H_{10}$	178.2358	Phenanthrene (c)	+27.3	+114.2	(1)
$C_{14}H_{10}$	178.2358	Phenanthrene (g)	+48.4	+202.5	(1)
$C_{14}H_{18}N_2O_2$	246.3118	Valylphenylalanyl anhydride (c)	-94.3	-394.6	(1)
$C_{14}H_{19}N_3O_4$	293.3252	Glycylalanyl phenylalanine (c)	-222.0	-928.8	(1)
$C_{14}H_{10}N_2O_3$	264.3271	Valylphenylalanine (c)	-183.5	-767.8	(1)
$C_{14}H_{20}O_9$	332.3101	Rhamnose triacetate (c)	-455.4	-1905.4	(1)
$C_{14}H_{23}N_3O_{10}$	393.3535	Diethylenetriaminepentaacetic acid (c)	-531.8	-2225.1	(1)
$C_{14}H_{26}$	194.3633	1-Tetradecyne (g)	-9.82	-41.09	(4)
$C_{14}H_{28}$	196.3793	1-Tetradecene (g)	-49.33	-206.40	(4)
$C_{14}H_{28}O_2$	228.3781	Methyl tridecylate (liq)	-171.56	-717.81	(1)
$C_{14}H_{28}O_2$	228.3781	Myristic acid (c)	-199.21	-833.49	(1)
$C_{14}H_{28}O_2$	228.3781	Myristic acid (liq)	-188.5	-788.7	(1)
$C_{14}H_{30}$	198.3952	n-Tetradecane (liq)	-96.33	-403.04	(4)
$C_{14}H_{20}N_2O_4$	290.4062	Tetramethylene-1,4-diamine-sebacic acid adduct (c)	-317.9	-1330.1	(1)
$C_{15}H_{20}O_6$	296.3231	Tricyclobutyrin (liq)	-247.	-1033.	(1)
$C_{15}H_{26}O_6$	302.3709	Glyceryl tributyrate (liq)	-356.	-1490.	(1)
$C_{15}H_{28}$	208.3904	1-Pentadecyne (g)	-14.74	-61.67	(4)
$C_{15}H_{30}$	210.4064	1-Pentadecene (g)	-54.26	-227.02	(4)
$C_{15}H_{30}O_2$	242.4051	Methyl myristate (liq)	-177.80	-743.92	(1)
$C_{15}H_{30}O_4$	274.4040	Glyceryl-1-laurate (c)	-277.46	-1160.89	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	Enthalpy of Formation kJ mol^{-1}	Ref
$C_{15}H_{30}O_4$	274.4040	Glyceryl-2-Laurate (c)	-275.48	-1152.61	(1)
$C_{15}H_{32}$	212.4223	n-Pentadecane (liq)	-102.44	-428.61	(4)
$C_{16}H_{10}$	202.2581	Fluoranthene (c)	+45.75	+191.42	(1)
$C_{16}H_{10}$	202.2581	Pyrene (c)	+27.44	+114.81	(1)
$C_{16}H_{10}N_2O_2$	262.2703	Indigotin (c)	-32.	-134.	(1)
$C_{16}H_{11}NO_2$	249.2716	Benzalhippuric acid azlactone (c)	-30.5	-127.6	(1)
$C_{16}H_{12}N_2O_4$	296.2850	Isatide (c)	-139.	-582.	(1)
$C_{16}H_{13}NO_3$	267.2869	Benzalhippuric acid (c)	-102.6	-429.3	(1)
$C_{16}H_{15}NO_3$	269.3029	Benzoylphenylalanine (c)	-129.6	-542.2	(1)
$C_{16}H_{22}O_{11}$	390.3471	Galactose pentaacetate (c)	-532.8	-2229.2	(1)
$C_{16}H_{22}O_{11}$	390.3471	Glucose pentaacetate (c)	-532.1	-2226.3	(1)
$C_{16}H_{30}$	222.4175	1-Hexadecyne (g)	-19.56	-81.84	(4)
$C_{16}H_{32}$	224.4334	1-Hexadecene (g)	-59.18	-247.61	(4)
$C_{16}H_{32}O_2$	256.4322	Methyl pentadecylate (liq)	-184.35	-771.32	(1)
$C_{16}H_{32}O_2$	256.4322	Palmitic acid (c)	-213.10	-891.61	(1)
$C_{16}H_{32}O_2$	256.4322	Palmitic acid (liq)	-200.4	-838.5	(1)
$C_{16}H_{34}$	226.4494	n-Hexadecane (liq)	-108.53	-454.09	(4)
$C_{17}H_{19}NO_2$	269.3465	Ethyl β-anilino-β-phenyl propionate (c)	-82.8	-346.4	(1)
$C_{17}H_{21}NO_4$	303.3612	Morphine monohydrate (c)	-170.1	-711.7	(1)
$C_{17}H_{34}O_4$	302.4581	Glyceryl-1-myristate (c)	-292.31	-1223.03	(1)
$C_{17}H_{34}O_4$	302.4581	Glyceryl-2-myristate (c)	-289.89	-1212.90	(1)
$C_{17}H_{32}$	236.4446	1-Heptadecyne (g)	-24.59	-102.38	(4)
$C_{17}H_{34}$	238.4605	1-Heptadecene (g)	-64.09	-268.15	(4)
$C_{17}H_{36}$	240.4765	n-Heptadecane (liq)	-114.64	-479.65	(4)
$C_{18}H_{12}$	228.2963	1,2-Benzanthracene (c)	+41.2	+172.4	(1)
$C_{18}H_{12}$	228.2963	3,4-Benzphenanthrene (c)	+44.5	+186.2	(1)
$C_{18}H_{12}$	228.2963	Chrysene (c)	+35.0	+146.4	(1)
$C_{18}H_{12}$	228.2963	Naphthacene (c)	+38.3	+160.2	(1)
$C_{18}H_{12}$	228.2963	Triphenylene (c)	+33.72	+141.08	(1)
$C_{18}H_{15}O_4P$	326.2916	Triphenyl phosphate (c)	-181.	-757.	(1)
$C_{18}H_{18}N_2O_2$	294.3564	Phenylalanyl anhydride (c)	-69.3	-290.0	(1)
$C_{18}H_{23}NO_4$	317.3883	Codeine monohydrate (c)	-151.2	-632.6	(1)
$C_{18}H_{26}O_6$	338.4043	Tricyclovalerin (liq)	-270.	-1130.	(1)
$C_{18}H_{32}O_{16}$	504.4461	Melezitose (c)	-815.	-3410.	(1)
$C_{18}H_{32}O_{16}$	504.4461	Raffinose (c)	-761.	-3184.	(1)
$C_{18}H_{34}$	250.4717	1-Octadecyne (g)	-29.50	-123.43	(4)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	Enthalpy of Formation kJ mol^{-1}	Ref
$C_{18}H_{34}O_2$	282.4705	Elaidic acid (c)	-217.7	-910.9	(1)
$C_{18}H_{34}O_2$	282.4705	Oleic acid (c)	-187.2	-783.2	(1)
$C_{18}H_{34}O_2$	282.4705	Oleic acid (liq)	-178.9	-748.5	(1)
$C_{18}H_{36}$	252.4876	1-Octadecene (g)	-69.02	-288.78	(4)
$C_{18}H_{36}O_2$	284.4864	Stearic acid (c)	-226.47	-947.55	(1)
$C_{18}H_{36}O_2$	284.4864	Stearic acid (liq)	-212.5	-889.1	(1)
$C_{18}H_{38}$	254.5036	n-Octadecane (liq)	-120.74	-505.18	(4)
$C_{18}H_{42}O_{21}$	594.5228	Raffinose pentahydrate (c)	-1122.	-4694.	(1)
$C_{19}H_{21}NO_3$	311.3841	Thebaine (c)	+63.0	-253.6	(1)
$C_{19}H_{22}N_2O$	294.4000	Cinchonidine (c)	+7.1	+29.7	(1)
$C_{19}H_{22}N_2O$	294.4000	Cinchonine (c)	+7.4	+31.0	(1)
$C_{19}H_{24}N_2O$	296.4159	Cinchonamine (c)	-10.4	-43.5	(1)
$C_{19}H_{25}N_3O_4$	359.4288	Cinchonamine nitrate (c)	-79.9	-334.3	(1)
$C_{19}H_{26}O_2$	286.4179	Δ4-Androstene-3,17-dione (c)	-103.	-431.	(1)
$C_{19}H_{28}O_2$	288.4338	5α-Androstane-3,17-dione (c)	-130.	-544.	(1)
$C_{19}H_{28}O_2$	288.4338	Δ5-Androstene-3β-ol-17-one (c)	-107.	-448.	(1)
$C_{19}H_{28}O_2$	288.4338	Δ4-Androstene-3-one-17β-ol (c)	-94.	-393.	(1)
$C_{19}H_{30}O_2$	290.4498	5α-Androstane-3α-ol-17-one (c)	-162.	-578.	(1)
$C_{19}H_{30}O_2$	290.4498	5α-Androstane-3β-ol-17-one (c)	-152.	-636.	(1)
$C_{19}H_{30}O_2$	290.4498	5α-Androstane-3-one-17β-ol (c)	-120.	-502.	(1)
$C_{19}H_{32}$	260.4669	5α-Androstane (c)	-75.	-314.	(1)
$C_{19}H_{36}$	264.4988	1-Nonadecyne (g)	-34.43	-144.06	(4)
$C_{19}H_{36}O_2$	296.4976	Methyl elaidate (liq)	-175.8	-735.5	(1)
$C_{19}H_{36}O_2$	296.4976	Methyl oleate (liq)	-174.2	-728.9	(1)
$C_{19}H_{38}$	266.5147	1-Nonadecene (g)	-73.94	-309.36	(4)
$C_{19}H_{38}O_4$	330.5123	Glyceryl-1-palmitate (c)	-306.28	-1281.48	(1)
$C_{19}H_{38}O_4$	330.5123	Glyceryl-2-palmitate (c)	-303.23	-1268.71	(1)
$C_{19}H_{40}$	268.5306	n-Nonadecane (liq)	-126.84	-530.70	(4)
$C_{20}H_{12}$	252.3186	Perylene (c)	+43.69	+182.8	(1)
$C_{20}H_{21}NO_4$	339.3947	Papaverine (c)	-120.2	-502.9	(1)
$C_{20}H_{24}N_2O_2$	324.4265	Quinidine (c)	-38.3	-160.2	(1)
$C_{20}H_{24}N_2O_2$	324.4265	Quinine (c)	-37.1	-155.2	(1)
$C_{20}H_{27}NO_{11}$	457.4383	Amygdalin (c)	-455.	-1904.	(1)
$C_{20}H_{38}$	278.5259	1-Eicosyne (g)	-39.36	-164.68	(4)
$C_{20}H_{40}$	280.5418	1-Eicosene (g)	-78.87	-329.99	(4)
$C_{20}H_{40}O_2$	312.5406	Arachidic acid (c)	-241.82	-1011.77	(1)

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TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	kJ mol⁻¹	Ref
$C_{20}H_{40}O_2$	312.5406	Arachidic acid (liq)	-224.6	-939.7	(1)
$C_{20}H_{42}$	282.5577	n-Eicosane (liq)	-132.94	-556.22	(4)
$C_{21}H_{16}N_2$	188.2747	Lophine (c)	+65.	+272.	(1)
$C_{21}H_{18}N_2$	298.3910	Amarine (c)	+63.	+264.	(1)
$C_{21}H_{19}N_2O_5$	307.3987	Amarine heminhydrate (c)	+29.	+121.	(1)
$C_{21}H_{22}N_2O_2$	334.4217	Strychnine (c)	-41.0	-171.5	(1)
$C_{21}H_{28}O_5$	360.4543	Δ4-Pregnene-3,11,20-trione-17α,21-diol (c)	-255.	-1067.	(1)
$C_{21}H_{30}O_2$	314.4721	Δ4-Pregnene-3,20-dione (c)	-132.	-552.	(1)
$C_{21}H_{30}O_3$	330.4715	Δ4-Pregnene-3,20-dione-21-ol (c)	-124.	-519.	(1)
$C_{21}H_{30}O_5$	362.4703	Δ4-Pregnene-3,20-dione-11β,17α,21-triol (c)	-256.	-1071.	(1)
$C_{21}H_{42}O_4$	358.5665	Glyceryl-1-stearate (c)	-319.64	-1337.37	(1)
$C_{21}H_{42}O_4$	358.5665	Glyceryl-2-stearate (c)	-315.80	-1321.31	(1)
$C_{22}H_{23}NO_7$	413.4311	Narcotine (c)	-210.9	-882.4	(1)
$C_{22}H_{42}O_2$	338.5788	Brassidic acid (c)	-214.	-895.	(1)
$C_{22}H_{42}O_2$	338.5788	Erucic acid (c)	-207.	-866.	(1)
$C_{22}H_{44}O_2$	340.5948	Behenic acid (c)	-235.	-983.	(1)
$C_{22}H_{44}O_4$	372.5936	13,14-Dihydroxybehenic acid (c)	-337.	-1410.	(1)
$C_{23}H_{26}N_2O_4$	394.4747	Brucine (c)	-118.6	-496.2	(1)
$C_{23}H_{31}NO_{10}$	481.5042	Narceine dihydrate (c)	-421.2	-1762.3	(1)
$C_{24}H_{20}O_6$	404.4234	Glyceryl tribenzoate (c)	-214.	-895.	(1)
$C_{24}H_{24}N_2O_3$	388.4705	Anisine (c)	-51.	-213.	(1)
$C_{24}H_{40}O_{20}$	648.5744	Diamylose (c)	-850.	-3556.	(1)
$C_{24}H_{42}O_6$	426.5987	5β-Cholan-24-oic acid-3α,7α,12α-triol monohydrate (c)	-288.	-1205.	(1)
$C_{24}H_{42}O_{21}$	666.5897	Stachyose (c)	-987.	-4130.	(1)
$C_{27}H_{46}O$	386.6671	Δ5-Cholestene-3β-ol (c)	-133.	-556.	(1)
$C_{28}H_{38}O_{19}$	678.6037	Celloblose octaacetate (c)	-902.5	-3776.1	(1)
$C_{28}H_{38}O_{19}$	678.6037	Lactose octaacetate (c)	-906.0	-3790.7	(1)
$C_{28}H_{38}O_{19}$	678.6037	Maltose octaacetate (c)	-904.5	-3784.4	(1)
$C_{28}H_{38}O_{19}$	678.6037	Sucrose octaacetate (c)	-901.9	-3773.5	(1)
$C_{28}H_{48}O$	400.6942	Δ5-Cholestene-3β-yl methyl ether (c)	-155.9	-652.3	(1)
$C_{28}H_{48}O$	400.6942	3:5-Cyclocholestan-6β-yl methyl ether (c)	-150.3	-628.9	(1)
$C_{32}H_{36}N_4O_2$	508.6693	Pyrroporphyrin (XV) monomethyl ester (c)	+88.6	-370.7	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol⁻¹	kJ mol⁻¹	Ref
$C_{32}H_{38}N_4$	478.6865	Aetioporphyrin (I) (c)	-1.8	-7.5	(1)
$C_{32}H_{38}N_4$	478.6865	Aetioporphyrin (II) (c)	+4.4	+18.4	(1)
$C_{33}H_{38}N_4O_2$	522.6964	γ-Phylloporphyrin monomethyl ester (c)	-87.3	-365.3	(1)
$C_{34}H_{34}N_4O_4$	562.6745	Protoporphyrin (c)	-120.6	-504.6	(1)
$C_{34}H_{36}N_4O_3$	548.6910	Phylloerythrin monomethyl ester (c)	-83.2	-348.1	(1)
$C_{34}H_{36}N_4O_3$	548.6910	Pyropheophorbide a monomethyl ester (c)	-84.8	-354.8	(1)
$C_{34}H_{36}N_4O_4$	564.6904	Verdoporphyrin dimethyl ester (c)	-143.3	-599.6	(1)
$C_{34}H_{36}N_4O_5$	580.6898	Pheopurpurin 18 monomethyl ester (c)	-230.8	-965.7	(1)
$C_{34}H_{38}N_4O_2$	534.7076	Desoxyphylloerythrin monomethyl ester (c)	-38.9	-162.8	(1)
$C_{34}H_{38}N_4O_4$	566.7064	Rhodoporphyrin (XV) dimethyl ester (c)	-122.2	-511.3	(1)
$C_{34}H_{38}N_4O_4$	566.7064	Rhodoporphyrin (XXI) dimethyl ester (c)	-123.9	-518.4	(1)
$C_{35}H_{38}N_4O_5$	594.7169	Chloroporphyrin e₅ dimethyl ester (c)	-103.3	-432.2	(1)
$C_{35}H_{40}N_4O_4$	580.7335	Chlorin e₄ dimethyl ester (c)	-144.9	-606.3	(1)
$C_{35}H_{40}N_4O_4$	580.7335	Chloroporphyrin e₄ dimethyl ester (c)	-154.2	-645.2	(1)
$C_{36}H_{36}N_4O_6$	620.7115	Methyl pheophorbide b (c)	-200.7	-839.7	(1)
$C_{36}H_{38}N_4O_4$	590.7287	Protoporphyrin dimethyl ester (c)	-122.1	-510.9	(1)
$C_{36}H_{38}N_4O_5$	606.7281	Methyl pheophorbide a (c)	-156.1	-653.1	(1)
$C_{36}H_{38}N_4O_5$	606.7281	Pheoporphyrin a₅ dimethyl ester (c)	-164.3	-687.4	(1)
$C_{36}H_{40}N_4O_6$	624.7434	Chlorin p₆ trimethyl ester (c)	-292.0	-1221.7	(1)
$C_{36}H_{42}N_4O_4$	594.7605	Mesoporphyrin (IX) dimethyl ester (c)	-196.4	-821.7	(1)
$C_{36}H_{44}N_2O_{10}$	664.7595	L(+)-Leucine methyl ester salt of (+)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3'') (c)	-540.	-2259.	
$C_{36}H_{44}N_2O_{10}$	664.7595	L(+)-Leucine methyl ester salt of (-)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3'') (c)	-531.	-2222.	
$C_{36}H_{46}N_4$	534.7948	Octaethylporphyrin (c)	-39.9	-166.9	(1)
$C_{36}H_{60}O_{30}$	972.8616	α-Tetamylose (c)	-1360.	-5690.	(1)
$C_{37}H_{40}N_4O_7$	652.7540	Dimethyl pheopurpurin 7 (c)	-245.8	-1028.4	(1)
$C_{37}H_{42}N_4O_6$	638.7705	Chlorin e₆ trimethyl ester (c)	-221.4	-926.3	(1)
$C_{37}H_{42}N_4O_6$	638.7705	Chloroporphyrin e₆ trimethyl ester (c)	-230.3	-963.6	(1)
$C_{39}H_{74}O_6$	639.0210	Glyceryl trilaurate (c)	-489.	-2046.	(1)
$C_{40}H_{46}N_4O_8$	710.8346	Coproporphyrin (I) tetramethyl ester (c)	-348.3	-1457.3	(1)
$C_{45}H_{86}O_6$	723.1836	Glyceryl trimyristate (c)	-520.	-2176.	(1)
$C_{47}H_{88}O_5$	733.2224	Glyceryl dibrassidate (c)	-472.	-1975.	(1)

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

Formula	Formula Weight	Name (state)	Enthalpy of Formation kcal mol^{-1}	Enthalpy of Formation kJ mol^{-1}	Ref
$C_{47}H_{88}O_5$	733.2224	Glyceryl dierucate (c)	-447.	-1870.	(1)
$C_{48}H_{54}N_4O_{16}$	942.9828	Iso-uroporphyrin (III) octamethyl ester (c)	-620.1	-2594.5	(1)
$C_{48}H_{80}O_{40}$	1297.1488	β-Hexamylose (c)	-1853.	-7753.	(1)
$C_{69}H_{128}O_6$	1053.7859	Glyceryl tribrassidate (c)	-625.	-2615.	(1)
$C_{69}H_{128}O_6$	1053.7859	Glyceryl trierucate (c)	-596.	-2494.	(1)

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25.3   TABLE I-B   COMPOUND NAME-FORMULA INDEX

TABLE I-B   COMPOUND NAME-FORMULA INDEX

Compound	Formula
Amarine	$C_{21}H_{18}N_2$
Amarine hemihydrate	$C_{21}H_{19}N_2O_{0.5}$
4-Amino-3-azido-5-ethyl-s-triazole	$C_4H_7N_7$
4-Amino-3-azido-5-methyl-s-triazole	$C_3H_5N_7$
4-Amino-3-azido-5-phenyl-s-triazole	$C_8H_7N_7$
4-Amino-3-azido-s-triazole	$C_2H_3N_7$
5-Aminobarbituric acid	see: Uramil
m-Aminobenzoic acid	$C_7H_7NO_2$
o-Aminobenzoic acid	$C_7H_7NO_2$
p-Aminobenzoic acid	$C_7H_7NO_2$
γ-Aminobutyric acid	$C_4H_9NO_2$
α-Aminocaproic acid	$C_6H_{13}NO_2$
γ-Aminocaproic acid	$C_6H_{13}NO_2$
δ-Aminocaproic acid	$C_6H_{13}NO_2$
ε-Aminocaproic acid	$C_6H_{13}NO_2$
5-Aminoenanthylic acid	$C_7H_{15}NO_2$
2-Aminoethane-1-sulfonic acid	$C_2H_7NO_3S$
3-Amino-5-methyl-1,2,4-triazole nitrate	$C_3H_7N_5O_3$
ω-Aminopelargonic acid	$C_9H_{19}NO_2$
5-Aminotetrazole	CH_3N_5
5-Aminotetrazole nitrate	$CH_4N_6O_3$
3-Amino-1,2,4-triazole	$C_2H_4N_4$
3-Amino-1,2,4-triazole nitrate	$C_2H_5N_5O_3$
δ-Aminovaleric acid	$C_5H_{11}NO_2$
Amygdalin	$C_{20}H_{27}NO_{11}$
5α-Androstane	$C_{19}H_{32}$
5α-Androstane-3,17-dione	$C_{19}H_{28}O_2$
5α-Androstane-3α-ol-17-one	$C_{19}H_{30}O_2$
5α-Androstane-3β-ol-17-one	$C_{19}H_{30}O_2$
5α-Androstane-3-one-17β-ol	$C_{19}H_{30}O_2$
Δ4-Androstene-3-one-17β-ol	$C_{19}H_{28}O_2$
Δ4-Androstene-3,17-dione	$C_{19}H_{26}O_2$
Δ5-Androstene-3β-ol-17-one	$C_{19}H_{28}O_2$
Androsterone	see: 5α-Androstane-3α-ol-17-one
Angelic acid	$C_5H_8O_2$
1,2-Anhydroglucose-3,5,6-triacetate	$C_{12}H_{18}O_8$
Aniline	C_6H_7N
Aniline nitrate	$C_6H_8N_2O_3$
Anisine	$C_{24}H_{24}N_2O_3$
Anisoyl glycine	$C_{10}H_{11}NO_4$
Anthracene	$C_{14}H_{10}$

TABLE I-B COMPOUND NAME-FORMULA INDEX

TABLE I-B COMPOUND NAME-FORMULA INDEX

TABLE I-B   COMPOUND NAME-FORMULA INDEX

Carbon trifluoride	CF_3
Carbonyl borane	CH_3BO
Carbonyl dibromide	CBr_2O
Carbonyl dichloride	CCl_2O
Carbonyl difluoride	CF_2O
Cellobiose	$C_{12}H_{22}O_{11}$
Cellobiose octaacetate	$C_{28}H_{38}O_{19}$
Chloral	C_2HCl_3O
Chloral hydrate	$C_2H_3Cl_3O_2$
Chlorin e_4 dimethyl ester	$C_{35}H_{40}N_4O_4$
Chlorin e_6 trimethyl ester	$C_{37}H_{42}N_4O_6$
Chlorin p_6 trimethyl ester	$C_{36}H_{40}N_4O_6$
Chloroacetyl chloride	$C_2H_2Cl_2O$
Chloroform	$CHCl_3$
Chloroporphyrin e_4 dimethyl ester	$C_{35}H_{40}N_4O_4$
Chloroporphyrin e_5 dimethyl ester	$C_{35}H_{38}N_4O_5$
Chloroporphyrin e_6 trimethyl ester	$C_{37}H_{42}N_4O_6$
Chlorotrifluoroethylene	C_2ClF_3
Chlorotrifluoromethane	$CClF_3$
5β-Cholan-24-oic acid-$3\alpha,7\alpha,12\alpha$-triol monohydrate	$C_{24}H_{42}O_6$
Δ_5-Cholestene-3β-ol	$C_{27}H_{46}O$
Δ_5-Cholestene-3β-yl methyl ether	$C_{28}H_{48}O$
Cholesterol	see: Δ_5-cholestene-3β-ol
Cholestryl methyl ether	see: Δ_5-Cholestene-3β-methyl ether
Cholic acid monohydrate	see: 5β-cholan-24-oic acid-$3\alpha,7\alpha,12x$-triol monohydrate
Chromium hexacarbonyl	C_6CrO_6
Chrysene	$C_{18}H_{12}$
Cinchonamine	$C_{19}H_{24}N_2O$
Cinchonamine nitrate	$C_{19}H_{25}N_3O_4$
Cinchonidine	$C_{19}H_{22}N_2O$
Cinchonine	$C_{19}H_{22}N_2O$
Citraconic acid	$C_5H_6O_4$
Citric acid, anhydrous	$C_6H_8O_7$
Citric acid monohydrate	$C_6H_{10}O_8$
Cobalt carbonate	$CCoO_3$
Cobaltous formate	$C_2H_2CoO_4$
Cobalt oxalate	C_2CoO_4
Codeine monohydrate	$C_{18}H_{23}NO_4$
Coniine	$C_8H_{17}N$

TABLE I-B   COMPOUND NAME-FORMULA INDEX

Compound	Formula
Coproporphyrin (I) tetramethyl ester	$C_{40}H_{45}N_4O_8$
Copper (II) acetate	$C_4H_6CuO_4$
Copper (II) formate	$C_2H_2CuO_4$
Copper (II) glycollate	$C_4H_6CuO_6$
Cortexone	see: Δ_4-pregnene-3,20-dione-21-ol
Cortisol	see: Δ_4-pregnene-3,20-dione-11β,17x,21-triol
Cortisone	see: Δ_4-pregnene-3,11,20-trione-17x,21-diol
Creatine	$C_4H_9N_3O_2$
Creatine hydrate	$C_4H_{11}N_3O_3$
Creatinine	$C_4H_7N_3O$
m-Cresol	C_7H_8O
o-Cresol	C_4H_8O
p-Cresol	C_7H_8O
cis-Crotonic acid	$C_4H_6O_2$
trans-Crotonic acid	$C_4H_6O_2$
3-Cyanopyridine	$C_6H_4N_2$
5-Cyanotetrazole	C_2HN_5
4-Cyanothiazole	$C_4H_2N_2S$
Cyclobutane	C_4H_8
3:5-Cyclocholestan-6β-yl methyl ether	$C_{28}H_{48}O$
Cycloheptane	C_7H_{14}
Cyclohexane	C_6H_{12}
Cyclooctane	C_8H_{16}
Cyclopentane	C_5H_{10}
Cyclopropane	C_3H_6
L-Cysteine	$C_3H_7NO_2S$
L-Cystine	$C_6H_{12}N_2O_4S_2$
n-Decane	$C_{10}H_{22}$
1,10-Decanediol	$C_{10}H_{22}O_2$
Decanoic acid	see: Capric acid
1-Decene	$C_{10}H_{20}$
1-Decyne	$C_{10}H_{18}$
trans-Dehydroandrosterone	see: Δ_5-Androstene-3β-ol-17-one
Dehydro-β-campholenolactone (dextrorotatory)	$C_{10}H_{16}O_2$
Dehydro-β-campholenolactone (inactive)	$C_{10}H_{16}O_2$
Desoxyamalic acid	$C_{12}H_{14}N_4O_6$
Desoxycorticosterone	see: Δ_4-Pregnene-3,20-dione-21-ol
Desoxyphylloerythrin monomethyl ester	$C_{34}H_{38}N_4O_2$
Diacetamide	$C_4H_7NO_2$
1,2,5,6-Diacetone mannitol	$C_{12}H_{22}O_6$
Diacetyl	see: 2,3-Butanedione
5-Diallylaminotetrazole	$C_7H_{11}N_5$

TABLE I-B COMPOUND NAME-FORMULA INDEX

Compound	Formula
Dialuric acid	$C_4H_4N_2O_4$
sym-Diaminoguanidine nitrate	$CH_8N_6O_3$
2,6-Diaminopyridine	$C_5H_7N_3$
Diamylose	$C_{24}H_{40}O_{20}$
1,2-Dibromo-1,2-dichloroethane	$C_2H_2Br_2Cl_2$
1,2-Dibromoethane	$C_2H_4Br_2$
1,2-Dibromo-1,1,2,2-tetrafluoroethane	CBr_2F_4
Dichloroacetic acid	$C_2H_2Cl_2O_2$
Dichloroacetyl chloride	C_2HCl_3O
1,2-Dichloro-1,2-difluoroethylene	$C_2Cl_2F_2$
Dichlorodifluoromethane	CCl_2F_2
1,1-Dichloroethane	$C_2H_4Cl_2$
1,2-Dichloroethane	$C_2H_4Cl_2$
1,1-Dichloroethylene	$C_2H_2Cl_2$
cis-1,2-Dichloroethylene	$C_2H_2Cl_2$
trans-1,2-Dichloroethylene	$C_2H_2Cl_2$
Diethylamine	$C_4H_{11}N$
Diethylamine nitrate	$C_4H_{12}N_2O_3$
2,2'-Diethyl-5,5'-azotriazole	$C_6H_{10}N_{10}$
Diethylbarbituric acid	$C_8H_{12}N_2O_3$
Diethylenetriaminepentaacetic acid	$C_{14}H_{23}N_3O_{10}$
Diethyl ether	$C_4H_{10}O$
Diethyl ketone	see: 3-Pentanone
Diethyl mercury	$C_4H_{10}Hg$
Diethyl tin	$C_4H_{12}Sn$
Diethyl zinc	$C_4H_{10}Zn$
Difluoroacetic acid	$C_2H_2F_2O_2$
1,1-Difluoro-2-chloroethylene	C_2HClF_2
1,1-Difluoroethane	$C_2H_4F_2$
2,2-Difluoroethanol	$C_2H_4F_2O$
1,1-Difluoroethylene	$C_2H_2F_2$
Diglycolamidic acid	$C_4H_7NO_4$
Diglycylglycine	$C_5H_{11}N_3O_4$
Dihydropyran, 4H	C_5H_8O
13,14-Dihydroxybehenic acid	$C_{22}H_{44}O_4$
1,2-Dihydroxybenzene	see: Pyrocatechol
1,3-Dihydroxybenzene	see: Resorcinol
1,4-Dihydroxybenzene	see: Hydroquinone

TABLE I-B COMPOUND NAME-FORMULA INDEX

TABLE I-B COMPOUND NAME-FORMULA INDEX

Compound Name	Formula
5,5-Dimethylhydantoin	$C_5H_8N_2O_2$
1,3-Dimethyl-5-iminotetrazole nitrate	$C_3H_8N_6O_3$
Dimethyl isophthalate	see: Dimethyl m-phthalate
Dimethyl maleate	$C_6H_8O_4$
Dimethyl malonate	$C_5H_8O_4$
Dimethyl mercury	C_2H_6Hg
Dimethyl oxalate	$C_4H_6O_4$
Dimethyl parabanic acid	$C_5H_6N_2O_3$
2,2-Dimethylpentane	C_7H_{16}
2,3-Dimethylpentane	C_7H_{16}
2,4-Dimethylpentane	C_7H_{16}
3,3-Dimethylpentane	C_7H_{16}
Dimethylpheopurpurin 7	$C_{37}H_{40}N_4O_7$
Dimethyl phthalate	see: Dimethyl o-phthalate
Dimethyl m-phthalate	$C_{10}H_{10}O_4$
Dimethyl o-phthalate	$C_{10}H_{10}O_4$
Dimethyl p-phthalate	$C_{10}H_{10}O_4$
2,2-Dimethylpropane	C_5H_{12}
2,3-Dimethylpyridine	C_7H_9N
2,4-Dimethylpyridine	C_7H_9N
2,5-Dimethylpyridine	C_7H_9N
2,6-Dimethylpyridine	C_7H_9N
3,4-Dimethylpyridine	C_7H_9N
3,5-Dimethylpyridine	C_7H_9N
Dimethyl tin	C_2H_8Sn
Dimethyl succinate	$C_6H_{10}O_4$
Dimethyl terephthalate	see: Dimethyl p-phthalate
1,4-Dimethyl-5-tetrazolone	$C_3H_6N_4O$
1,5-Dimethyltetrazole	$C_3H_6N_4$
Dimethyl zinc	C_2H_6Zn
1,3-Dioxane	$C_4H_8O_2$
1,4-Dioxane	$C_4H_8O_2$
Dioxindole	$C_8H_7NO_2$
Dipentaerythritol	$C_{10}H_{22}O_7$
Diphenyl disulfide	$C_{12}H_{10}S_2$
Diphenyl sulfide	$C_{12}H_{10}S$
Di-α-pyrrylketone	$C_9H_8N_2O$
Dipyrrylmethane	$C_9H_{10}N_2$
1,2-Di-(5-tetrazolyl)ethane	$C_4H_6N_8$
2,3-Dithiabutane	$C_2H_6S_2$
β,β'-Dithiodilactic acid	$C_6H_{10}O_4S_2$

TABLE I-B COMPOUND NAME-FORMULA INDEX

Compound name	Formula
Docosanoic acid	see: Behenic acid
n-Dodecane	$C_{12}H_{26}$
Dodecanoic acid	see: Lauric acid
1-Dodecene	$C_{12}H_{24}$
1-Dodecyne	$C_{12}H_{22}$
Dulcitol	$C_6H_{14}O_6$
n-Eicosane	$C_{20}H_{42}$
Eicosanoic acid	see: Arachidic acid
1-Eicosene	$C_{20}H_{40}$
1-Eicosyne	$C_{20}H_{38}$
Elaidic acid	$C_{18}H_{34}O_2$
Enanthic acid	$C_7H_{14}O_2$
ζ-Enantholactam	$C_7H_{13}NO$
Epiandrosterone	see: 5α-Androstane-3β-ol-17-one
Erucic acid	$C_{22}H_{42}O_2$
meso-Erythritol	see: meso-1,2,3,4-Butanetetrol
Erythritol diacetal	$C_8H_{14}O_4$
Erythritol diformal	$C_6H_{10}O_4$
Ethanal	see: Acetaldehyde
Ethane	C_2H_6
1,2-Ethanediol	$C_2H_6O_2$
1,2-Ethanedithiol	$C_2H_6S_2$
Ethanethiol	C_2H_6S
Ethanoic acid	see: Acetic acid
Ethanol	C_2H_6O
Ethenylbenzene	C_8H_8
Ethylacetylene	see: 1-Butyne
Ethyl alcohol	see: Ethanol
Ethylamine	C_2H_7N
Ethylamine nitrate	$C_2H_8N_2O_3$
Ethyl β-anilino-β-phenyl propionate	$C_{17}H_{19}NO_2$
Ethylbenzene	C_8H_{10}
Ethyl bromide	C_2H_5Br
Ethyl carbamate	$C_3H_7NO_2$
Ethyl chloride	C_2H_5Cl
Ethylcyclohexane	C_8H_{16}
Ethylcyclopentane	C_7H_{14}
Ethylene	C_2H_4
Ethylene carbonate	$C_3H_4O_3$
Ethylene chlorohydrin	C_2H_5ClO
Ethylenediamine	$C_2H_8N_2$

TABLE I-B COMPOUND NAME-FORMULA INDEX

TABLE I-B   COMPOUND NAME-FORMULA INDEX

Name	Formula
D-Gluconic acid-δ-lactone	$C_6H_{10}O_6$
D-Gluco-α,α-octonic acid-γ-lactone	$C_8H_{14}O_8$
α-D-Glucose	$C_6H_{12}O_6$
β-D-Glucose	$C_6H_{12}O_6$
α-D-Glucose hydrate	$C_6H_{14}O_7$
Glucose pentaacetate	$C_{16}H_{22}O_{11}$
L-Glutamic acid	$C_5H_9NO_4$
L-Glutamine	$C_5H_{10}N_2O_3$
Glutaric acid	$C_5H_8O_4$
Glyceraldehyde	$C_3H_6O_3$
Glycerol	see: 1,2,3-Propanetriol
Glyceryl-1-acetate	$C_5H_{10}O_4$
Glyceryl-1-benzoate	$C_{10}H_{12}O_4$
Glyceryl-2-benzoate	$C_{10}H_{12}O_4$
Glyceryl-1-caprate	$C_{13}H_{26}O_4$
Glyceryl-2-caprate	$C_{13}H_{26}O_4$
Glyceryl-1,3-diacetate	$C_7H_{12}O_5$
Glyceryl dibrassidate	$C_{47}H_{88}O_5$
Glyceryl dierucate	$C_{47}H_{88}O_5$
Glyceryl-1-laurate	$C_{15}H_{30}O_4$
Glyceryl-2-laurate	$C_{15}H_{30}O_4$
Glyceryl-1-myristate	$C_{17}H_{34}O_4$
Glyceryl-2-myristate	$C_{17}H_{34}O_4$
Glyceryl-1-palmitate	$C_{19}H_{38}O_4$
Glyceryl-2-palmitate	$C_{19}H_{38}O_4$
Glyceryl-1-stearate	$C_{21}H_{42}O_4$
Glyceryl-2-stearate	$C_{21}H_{42}O_4$
Glyceryl triacetate	$C_9H_{14}O_6$
Glyceryl tribenzoate	$C_{24}H_{20}O_6$
Glyceryl tribrassidate	$C_{69}H_{128}O_6$
Glyceryl tributyrate	$C_{15}H_{26}O_6$
Glyceryl trierucate	$C_{69}H_{128}O_6$
Glyceryl trilaurate	$C_{39}H_{74}O_6$
Glyceryl trimyristate	$C_{45}H_{86}O_6$
Glycine	$C_2H_5NO_2$
Glycine anhydride	$C_4H_6N_2O_2$
Glycine nitrate	$C_2H_6N_2O_5$
Glycol acetal	$C_4H_8O_2$
Glycolic acid	$C_2H_4O_3$
Glycylalanyl phenylalanine	$C_{14}H_{19}N_3O_4$
Glycylglycine	$C_4H_8N_2O_3$

TABLE I-B COMPOUND NAME-FORMULA INDEX

TABLE I-B COMPOUND NAME-FORMULA INDEX

Compound	Formula
Hexanoic acid	see: Caproic acid
1-Hexanol	$C_6H_{14}O$
1-Hexene	C_6H_{12}
1-Hexyne	C_6H_{10}
n-Hexyl alcohol	see: 1-Hexanol
Hippuric acid	$C_9H_9NO_3$
Hippurylglycine	$C_{11}H_{12}N_2O_4$
Hydantoic acid	$C_3H_6N_2O_3$
Hydantoin	$C_3H_4N_2O_2$
Hydrazodicarbamide	$C_2H_6N_4O_2$
5,5'-Hydrazotetrazole	$C_2H_4N_{10}$
Hydroquinone	$C_6H_6O_2$
Hydrosorbic acid	$C_6H_{10}O_2$
Hydroxyacetic acid	see: Glycolic acid
DL-β-Hydroxybutyric acid	$C_4H_8O_3$
3(a)-Hydroxy-trans-decalin-2(a) acetic acid lactone (boat form)	$C_{12}H_{18}O_2$
3(e)-Hydroxy-trans-decalin-2(e) acetic acid lactone (chair form)	$C_{12}H_{18}O_2$
Hydroxyisobutyric acid	$C_4H_8O_3$
5-Hydroxy-1-pentanal	$C_5H_{10}O_2$
L-Hydroxyproline	$C_5H_9NO_3$
8-Hydroxyquinoline	C_9H_7NO
5-Hydroxytetrazole	CH_2N_4O
Hydurilic acid	$C_8H_6N_4O_6$
Hypoxanthine	$C_5H_4N_4O$
Imidazole	$C_3H_4N_2$
Indigotin	$C_{16}H_{10}N_2O_2$
Indole	C_8H_7N
Iodoform	CHI_3
Iron (II) carbonate	$CFeO_3$
Iron pentacarbonyl	C_5FeO_5
Isatide	$C_{16}H_{12}N_2O_4$
Isatin	$C_8H_5NO_2$
Isobutene	see: 2-Methyl propene
Isobutyl alcohol	see: 2-Methyl-1-propanol
Isobutylamine	$C_4H_{11}N$
DL-Isoleucine	$C_6H_{13}NO_2$
L-Isoleucine	$C_6H_{13}NO_2$
Isopentane	see: 2-Methylbutane
Isophthalic acid	see: m-Phthalic acid

TABLE I-B   COMPOUND NAME-FORMULA INDEX

Isopropyl alcohol	see: 2-Propanol
Isopropylamine	C_3H_9N
Isopropylbenzene	C_9H_{12}
Isoquinoline	C_9H_7N
L-Isoserine	$C_3H_7NO_3$
Isouric acid	$C_5H_4N_4O_3$
Iso-uroporphyrin (II) octamethyl ester	$C_{48}H_{54}N_4O_{16}$
Itaconic acid	$C_5H_6O_4$
α-Ketoglutaric acid	$C_5H_6O_5$
γ-Ketovaleric acid	see: Levulinic acid
D-Lactic acid	$C_3H_6O_3$
DL-Lactic acid	$C_3H_6O_3$
Lactide	$C_6H_8O_4$
β-Lactose	$C_{12}H_{22}O_{11}$
α-Lactose monohydrate	$C_{12}H_{24}O_{12}$
Lactose octaacetate	$C_{28}H_{38}O_{19}$
Lauric acid	$C_{12}H_{24}O_2$
Lead acetate	$C_4H_6O_4Pb$
Lead formate	$C_2H_2O_4Pb$
D-Leucine	$C_6H_{13}NO_2$
DL-Leucine	$C_6H_{13}NO_2$
L-Leucine	$C_6H_{13}NO_2$
Leucine anhydride	$C_{12}H_{22}N_2O_2$
L(+)-Leucine methyl ester salt of (-)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3')	$C_{36}H_{44}N_2O_{10}$
L(+)-Leucine methyl ester salt of (+)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3')	
DL-Leucylglycine	$C_8H_{16}N_2O_3$
Leucylglycylglycine	$C_{10}H_{19}N_3O_4$
Levoglucosan	$C_6H_{10}O_5$
Levoglucosan triacetate	$C_{12}H_{16}O_8$
Levulinic acid	$C_5H_8O_3$
Levulinic lactone	$C_5H_6O_2$
Lophine	$C_{21}H_{16}N_2$
DL-Lysine	$C_6H_{14}N_2O_2$
Maleic acid	$C_4H_4O_4$
Maleic anhydride	$C_4H_2O_3$
DL-Malic acid	$C_4H_6O_5$
L-Malic acid	$C_4H_6O_5$

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TABLE I-B COMPOUND NAME-FORMULA INDEX

Compound	Formula
Malonamide	$C_3H_6N_2O_2$
Malonic acid	$C_3H_4O_4$
Maltose	$C_{12}H_{22}O_{11}$
β-Maltose monohydrate	$C_{12}H_{24}O_{12}$
Maltose octaacetate	$C_{28}H_{38}O_{19}$
DL-Mandelic acid	$C_9H_8O_3$
L-Mandelic acid	$C_8H_8O_3$
Manganese acetate	$C_4H_6MnO_4$
Manganese carbonate	$CMnO_3$
Manganese formate	$C_2H_2MnO_4$
D-Mannitol	$C_6H_{14}O_6$
Mannitol triacetal	$C_{12}H_{20}O_6$
Mannitol triformal	$C_9H_{14}O_6$
D-Mannonic-1,4-3,6-dilactone	$C_6H_6O_6$
D-Mannonic acid-γ-lactone	$C_6H_{10}O_6$
D-Mannose	$C_6H_{12}O_6$
Melamine	$C_3H_6N_6$
Melezitose	$C_{18}H_{32}O_{16}$
Mesaconic acid	$C_5H_6O_4$
Mesoporphyrin (IX) dimethyl ester	$C_{36}H_{42}N_4O_4$
Mesoxalic acid	$C_3H_4O_6$
Methanal	see: Formaldehyde
Methane	CH_4
Methanethiol	CH_4S
Methanoic acid	see: Formic acid
Methanol	CH_4O
L-Methionine	$C_5H_{11}NO_2S$
5-Methoxytetrazole	$C_2H_4N_4O$
Methyl acetate	$C_3H_6O_2$
Methylacetylene	see: Propyne
Methyl alcohol	see: Methanol
Methyl allantoin	$C_5H_8N_4O_3$
Methylamine	CH_5N
Methylamine nitrate	$CH_6N_2O_3$
1-Methyl-5-aminotetrazole	$C_2H_5N_5$
2-Methyl-5-aminotetrazole	$C_2H_5N_5$
5-Methylaminotetrazole	$C_2H_5N_5$
N-Methylaniline	C_7H_9N
Methylbenzene	see: Toluene
Methyl benzoate	$C_8H_8O_2$
Methyl bromide	CH_3Br

TABLE I-B COMPOUND NAME-FORMULA INDEX

TABLE I-B   COMPOUND NAME-FORMULA INDEX

TABLE I-B COMPOUND NAME-FORMULA INDEX

TABLE I-B COMPOUND NAME-FORMULA INDEX

TABLE I-B COMPOUND NAME-FORMULA INDEX

Compound	Formula
Phenol	C_6H_6O
Phenoxyacetic acid	$C_8H_8O_3$
Phenylacetic acid	$C_8H_8O_2$
DL-Phenylalanine	$C_9H_{11}NO_2$
L-Phenylalanine	$C_9H_{11}NO_2$
Phenylalanyl anhydride	$C_{18}H_{18}N_2O_2$
Phenylalanine N-carboxylic acid anhydride	$C_{10}H_9NO_3$
DL-Phenylalanine-N-carboxylic acid dimethyl ester	$C_{12}H_{15}NO_4$
1-Phenyl-5-aminotetrazole	$C_7H_7N_5$
5-Phenylaminotetrazole	$C_7H_7N_5$
DL-Phenylglyceric acid	$C_9H_{10}O_4$
α-Phenyl glycine	$C_8H_9NO_2$
N-Phenyl glycine	$C_8H_9NO_2$
Phenylglyoxylic acid	$C_8H_6O_3$
1-Phenyl-5-hydroxytetrazole	$C_7H_6N_4O$
Phenyl methyl sulfide	C_7H_8S
1-Phenyl-5-methyltetrazole	$C_8H_8N_4$
2-Phenyl-5-methyltetrazole	$C_8H_8N_4$
α-Phenylpyrrole	$C_{10}H_9N$
N-Phenylpyrrole	$C_{10}H_9N$
1-Phenyltetrazole	$C_7H_6N_4$
5-Phenyltetrazole	$C_7H_6N_4$
4-Phenyluracil	$C_{10}H_8N_2O_2$
Pheoporphyrin a_5 dimethyl ester	$C_{36}H_{38}N_4O_5$
Pheopurpurin 18 monomethyl ester	$C_{34}H_{36}N_4O_5$
Phthalamide	$C_8H_8N_2O_2$
Phthalic acid	see: o-Phthalic acid
m-Phthalic acid	$C_8H_6O_4$
o-Phthalic acid	$C_8H_6O_4$
p-Phthalic acid	$C_8H_6O_4$
Phylloerythrin monomethyl ester	$C_{34}H_{36}N_4O_3$
γ-Phylloporphyrin monomethyl ester	$C_{33}H_{38}N_4O_2$
Phyllopyrrole	$C_9H_{15}N$
Picolinic acid	$C_6H_5NO_2$
Piperazine	$C_4H_{10}N_2$
Piperazine hexahydrate	$C_4H_{22}N_2O_6$
Piperidine	$C_5H_{11}N$
α-Piperidone	C_5H_9NO
Δ_4-Pregnene-3,20-dione	$C_{21}H_{30}O_2$
Δ_4-Pregnene-3,20-dione-21-ol	$C_{21}H_{30}O_3$

TABLE I-B COMPOUND NAME-FORMULA INDEX

Compound	Formula
Δ_4-Pregnene-3,20-dione-11β,17α,21-triol	$C_{21}H_{30}O_5$
Δ_4-Pregnene-3,11,20-trione-17β,21-diol	$C_{21}H_{28}O_5$
Progesterone	see: Δ_4-Pregnene-3,20-dione
DL-Proline	$C_5H_9NO_2$
Propadiene	C_4H_3
1-Propanal	see: n-Propionaldehyde
Propane	C_3H_8
1,2-Propanediamine	$C_3H_{10}N_2$
1,2-Propanediol	$C_3H_8O_2$
1,3-Propanediol	$C_3H_8O_2$
1,3-Propanedithiol	$C_3H_8S_2$
1-Propanethiol	C_3H_8S
1,2,3-Propanetriol	$C_3H_8O_3$
Propanoic acid	see: Propionic acid
1-Propanol	C_3H_8O
2-Propanol	C_3H_8O
Propanone	C_3H_6O
Propene	C_3H_6
β-Propiolactone	$C_3H_4O_2$
n-Propionaldehyde	C_3H_6O
Propionamide	C_3H_7NO
Propionic acid	$C_3H_6O_2$
n-Propyl alcohol	see: 1-Propanol
n-Propylamine	C_3H_9N
n-Propylbenzene	C_9H_{12}
n-Propylcyclohexane	C_9H_{18}
n-Propylcyclopentane	C_8H_{16}
Propylene	see: Propene
Propylene glycol	see: 1,2- and 1,3-Propanediol
Propyne	C_3H_4
Protoporphyrin	$C_{34}H_{34}N_4O_4$
Protoporphyrin dimethyl ester	$C_{36}H_{38}N_4O_4$
Pseudouric acid	$C_5H_6N_4O_4$
Pyrazine	$C_4H_4N_2$
Pyrazole	$C_3H_4N_2$
Pyrene	$C_{16}H_{10}$
Pyridazine	$C_4H_4N_2$
Pyridine	C_5H_5N
Pyrimidine	$C_4H_4N_2$
Pyrocatechol	$C_6H_6O_2$
Pyromucic acid	see: 2-Furoic acid

TABLE I-B COMPOUND NAME-FORMULA INDEX

Compound	Formula
Pyropheophorbide a monomethyl ester	$C_{34}H_{36}N_4O_3$
Pyrrolaldehyde	C_5H_5NO
Pyrrolaldoxime	$C_5H_6N_2O$
Pyrrole	C_4H_5N
Pyrrolidine	C_4H_9N
α-Pyrrolidone	C_4H_7NH
Pyrroporphyrin (XV) monomethyl ester	$C_{32}H_{36}N_4O_2$
Pyruvic acid	$C_3H_4O_3$
Pyvurile	see: Methyl allantoin
Quinaldine	$C_{10}H_9N$
Quinidine	$C_{20}H_{24}N_2O_2$
Quinine	$C_{20}H_{24}N_2O_2$
Quinoline	C_9H_7N
Raffinose	$C_{18}H_{32}O_{16}$
Raffinose pentahydrate	$C_{18}H_{42}O_{21}$
Resorcinol	$C_6H_6O_2$
β-L-Rhamnose	$C_6H_{12}O_5$
α-L-Rhamnose monohydrate	$C_6H_{14}O_6$
Rhamnose triacetate	$C_{14}H_{20}O_9$
Rhodoporphyrin (XV) dimethyl ester	$C_{34}H_{38}N_4O_4$
Rhodoporphyrin (XXI) dimethyl ester	$C_{34}H_{38}N_4O_4$
β-D-Ribose	$C_5H_{10}O_5$
Saccharinic acid lactone	$C_6H_{10}O_5$
Salicylaldehyde	$C_7H_6O_2$
Salicylic acid	$C_7H_6O_3$
Sarcosine	$C_3H_7NO_2$
Sarcosine-N-carboxylic acid anhydride	$C_4H_5NO_3$
L-Serine	$C_3H_7NO_3$
Serine anhydride	$C_6H_{10}N_2O_4$
Serylserine	$C_6H_{12}N_2O_5$
Skatole	C_9H_9N
Silver acetate	$C_2H_3AgO_2$
Silver carbonate	CAg_2O_3
Silver oxalate	$C_2Ag_2O_4$
Sorbic acid	$C_6H_8O_2$
L-Sorbose	$C_6H_{12}O_6$
Spiropentane	C_5H_8
Stachyose	$C_{24}H_{42}O_{21}$
Stearic acid	$C_{18}H_{36}O_2$
Strychnine	$C_{21}H_{22}N_2O_2$
Styrene	see: Ethenylbenzene

TABLE I-B COMPOUND NAME-FORMULA INDEX

TABLE I-B COMPOUND NAME-FORMULA INDEX

Tri-n-butyl phosphine oxide	$C_{12}H_{27}OP$
Trichloroacetic acid	$C_2HCl_3O_2$
Trichloroacetyl chloride	C_2Cl_4O
1,1,2-Trichloroethane	$C_2H_3Cl_3$
Trichloroethylene	C_2HCl_3
1,1,2-Trichloro-2,2,1-trifluoroethane	$C_2Cl_3F_3$
Tricyclobutyrin	$C_{15}H_{20}O_6$
Tricyclovaler,in	$C_{18}H_{26}O_6$
n-Tridecane	$C_{13}H_{28}$
1-Tridecene	$C_{13}H_{26}$
1-Tridecyne	$C_{13}H_{24}$
Triethoxyborane	$C_6H_{15}BO_3$
Triethoxysilane	$C_6H_{16}O_3Si$
Triethylamine	$C_6H_{15}N$
Triethylamine nitrate	$C_6H_{16}N_2O_3$
Triethylboron	$C_6H_{15}B$
Triethylenediamine	$C_6H_{12}N_2$
Triethyl phosphate	$C_6H_{15}O_4P$
Triethylsilane	$C_6H_{16}Si$
1,1,1-Trifluoroethane	$C_2H_3F_3$
1,1,2-Trifluoroethane	$C_2H_3F_3$
2,2,2-Trifluoroethanol	$C_2H_3F_3O$
Triglycylglycine	$C_8H_{14}N_4O_5$
DL-Trihydroxyglutaric acid	$C_5H_8O_7$
Triisobutyl phosphate	$C_{12}H_{27}O_4P$
Trimethoxyborane	$C_3H_9BO_3$
Trimethoxysilane	$C_3H_{10}O_3Si$
Trimethyl aluminum	C_3H_9Al
Trimethylamine	C_3H_9N
Trimethylamine nitrate	$C_3H_{10}N_2O_3$
1,2,3-Trimethylbenzene	C_9H_{12}
1,2,4-Trimethylbenzene	C_9H_{12}
1,3,5-Trimethylbenzene	C_9H_{12}
Trimethyl boron	C_3H_9B
2,2,3-Trimethylbutane	C_7H_{16}
Trimethylene oxide	see: Oxacyclobutane
2,4,5-Trimethyl-3-ethylpyrrole	see: Phyllopyrrole
Trimethyl gallium	C_3H_9Ga
2,2,3-Trimethylpentane	C_8H_{18}
2,2,4-Trimethylpentane	C_8H_{18}
2,3,3-Trimethylpentane	C_8H_{18}

TABLE I-B COMPOUND NAME-FORMULA INDEX

25.4 Table II. Enthalpies of Formation of Organic Polymers at 298.15 K

formula (repeating unit)	formula weight (g mol^{-1})	name (state)	Enthalpy of formation kcal mol^{-1}	kJ mol^{-1}	Ref.
[-CH$_{1.891}$-]$_n$	13.9172	Mineral oil (liq)	-5.5	-23.0	[1]
[-CH$_2$-]$_n$	14.0271	Polymethylene (s)	-6.99	-29.25	[2]
[-CH$_2$O-]$_n$	30.0265	Polyoxymethylene (s)	-40.93	-171.25	[2]
[-C$_2$H$_2$Cl$_2$-]$_n$	96.9442	Poly-1,1-dichloroethylene (s)	-24.0	-100.4	[3]
[-C$_2$H$_2$F$_2$-]$_n$	64.0350	Polyvinylidene fluoride	-114.58	-479.40	[4]
[-C$_2$H$_3$Cl-]$_n$	62.4992	Polyvinylchloride (s)	-22.5	-94.1	[3]
[-CF$_2$CF$_2$-]$_n$	100.0159	Teflon, polytetrafluoroethylene (s)	-197.82	-827.68	[5]
[-CH$_2$CH$_2$-]$_n$	28.0542	Polyethylene (s)	-13.50	-56.48	[2,6]
[-C$_3$O$_2$-]$_n$	68.0322	Poly(carbon suboxide) (s)	-56.6	-236.8	[7]
[-C$_3$H$_5$NO-]$_n$	71.0794	Sarcosine polypeptide (s)	-53.2	-222.6	[8]
[-C$_3$H$_6$-]$_n$	42.0813	Polypropylene (s)	-20.02	-83.76	[6]
[-C$_3$H$_6$O-]$_n$	58.0807	Polyvinyl methyl ether (s)	-48.92	-204.68	[22]
[-C$_4$H$_6$-]$_n$	54.0924	Polybutadiene (s)	+3.3	+13.8	[9]
[-C$_4$H$_8$-]$_n$	56.1084	Poly(butene-1) (s)	-24.68	-103.26	[6]
[-C$_4$H$_8$-]$_n$	56.1084	Polyisobutylene (s)	-21.18	-88.62	[10,11]
[-C$_4$H$_8$O-]$_n$	72.1078	Polyvinyl ethyl ether (s)	-56.92	-238.15	[22]
[-C$_4$H$_8$O$_2$S-]$_n$	120.1712	But-1-ene polysulfone (s)	-100.08	-418.73	[12]
[-C$_4$H$_8$O$_2$S-]$_n$	120.1712	Isobutene polysulfone (s)	-100.46	-420.32	[12]
[-C$_4$H$_8$O$_2$S-]$_n$	120.1712	cis-But-2-ene polysulfone (s)	-101.50	-424.68	[12]
[-C$_4$H$_8$O$_2$S-]$_n$	120.1712	trans-But-2-ene polysulfone (s)	-101.36	-424.09	[12]
[-C$_5$H$_8$-]$_n$	68.1195	Polyisoprene, purified rubber (s)	-6.24	-26.11	[23,24]
[-C$_6$H$_{10}$O$_5$-]$_n$	162.1436	Cellulose (s)	-229.7	-961.1	[13]
[-C$_6$H$_{10}$O$_5$-]$_n$	162.1436	Glycogen (s)	-225.	-941.	[15,16]

Enthalpies of Formation of Organic Polymers at 298.15 K (Cont'd)

formula (repeating unit)	formula weight (g mol^{-1})	name (state)	Enthalpy of formation kcal mol^{-1}	Enthalpy of formation kJ mol^{-1}	Ref.
[-C$_6$H$_7$N$_3$O$_{11}$-]$_n$	297.1362	Trinitrocellulose (s)	-155.7	-651.4	[13]
[-C$_6$H$_8$N$_2$O$_9$-]$_n$	252.1387	Dinitrocellulose (s)	-179.9	-752.7	[13]
[-C$_6$H$_9$NO$_7$-]$_n$	207.1411	Mononitrocellulose (s)	-205.	-858.	[14]
[-C$_8$H$_8$-]$_n$	104.1530	Polystyrene (s) (isotactic, 40% crystalline)	+7.09	+29.66	[6]
[-C$_8$H$_8$-]$_n$	104.1530	Polystyrene (s) (isotactic, amorphous)	+7.99	+33.43	[6]
[-C$_8$H$_8$-]$_n$	104.1530	Polystyrene (s) (atactic, amorphous)	+8.25	+34.52	[6,17]
[-C$_8$H$_8$O-]$_n$	120.1524	Poly(2,6-dimethylphenylene ether) (s)	-31.88	-133.39	[6]
[-C$_8$H$_{12}$O$_6$-]$_n$	204.1812	Cellulose monoacetate (s)	-278.	-1163.	[19]
[-C$_9$H$_{10}$-]$_n$	118.1800	Poly(α-methylstyrene) (s)	+7.88	+32.97	[6]
[-C$_9$H$_9$NO-]$_n$	147.1782	Phenylalanine polypeptide (s) (benzene soluble)	-49.6	-207.5	[8]
[-C$_9$H$_9$NO-]$_n$	147.1782	Phenylalanine polypeptide (s) (benzene insoluble)	-53.1	-222.2	[8]
[-C$_{10}$H$_8$O$_4$-]$_n$	192.1729	Mylar, Melinex, Terylene film, polyester of ethylene glycol and terephthalic acid (s)	-161.1	-674.0	[20,21]
[-C$_{10}$H$_{14}$O$_7$-]$_n$	246.2189	Cellulose diacetate (s)	-326.	-1364.	[18]
[-C$_{12}$H$_8$-]$_n$	152.1976	Polyacenaphthylene (s)	+27.13	+113.51	[6]
[-C$_{12}$H$_{16}$O$_8$-]$_n$	288.2565	Cellulose triacetate (s)	-377.	-1577.	[18]
[-C$_{16}$H$_{14}$O$_3$-]$_n$	254.2882	Poly(4,4'-dioxydiphenyl-2,2-propane carbonate) (s)	-103.26	-432.04	[6]

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25.5 Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K

formula (state)	formula weight (g mol^{-1})	name	Enthalpy of formation, $\Delta Hf°$ kcal mol^{-1}	kJ mol^{-1}	Ref.
Ag_2O (c)	231.7394	Silver oxide	-7.42	-31.04	[4]
Ag_2O_2 (c)	247.7388	Silver peroxide	-5.8	-24.3	[4]
Ag_2O_3 (c)	263.7382	Silver sesquioxide	8.1	33.9	[4]
AlO (g)	42.9809	Aluminum monoxide	21.8	91.2	[3]
$(AlO)_2$ (g)	85.9618	Aluminum monoxide, dimer	-94.	-393.	[3]
Al_2O (g)	69.9624	Dialuminum monoxide	-31.	-130.	[3]
Al_2O_3 (c,α)	101.9612	Aluminum oxide,α-Alumina, Corundum	-400.5	-1675.7	[3]
Al_2O_3 (c,γ)	101.9612	Aluminum oxide, γ-Alumina	-395.	-1653.	[3]
Al_2O_3 (c,δ)	101.9612	Aluminum oxide, δ-Alumina	-398.	-1665.	[3]
Al_2O_3 (c,κ)	101.9612	Aluminum oxide, κ-Alumina	-397.	-1661.	[3]
Al_2O_3 (c,ρ)	101.9612	Aluminum oxide, ρ-Alumina	-391.	-1636.	[3]
Al_2O_3 (amorp)	101.9612	Aluminum oxide	-390.	-1632.	[3]
AsO (g)	90.9210	Arsenic monoxide	16.72	69.96	[3]
As_2O_4 (c)	213.8408	Diarsenic tetroxide	-189.72	-793.79	[3]
As_2O_5 (c)	229.8402	Arsenic pentoxide	-221.05	-924.87	[3]
As_4O_6 (g)	395.6828	Arsenic trioxide	-289.0	-1209.2	[3]
As_4O_6 (c, octahedral)	395.6828	Arsenic trioxide, Arsenolite	-314.04	-1313.94	[3]
As_4O_6 (c, monoclinic)	395.6828	Arsenic trioxide, Claudetite	-313.0	-1309.6	[3]

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

formula (state)	formula weight (g mol^{-1})	name	Enthalpy of formation, $\Delta H_f°$ kcal mol^{-1}	kJ mol^{-1}	Ref.
BO (g)	26.8104	Boron monoxide	6.	25.	[3]
BO$_2$ (g)	42.8098	Boron dioxide	-71.8	-300.4	[3]
B$_2$O$_2$ (g)	53.6208	Diboron dioxide	-108.7	-454.8	[3]
B$_2$O$_3$ (g)	69.6202	Boric oxide	-201.67	-843.79	[3]
B$_2$O$_3$ (c)	69.6202	Boric oxide	-304.20	-1272.77	[3]
B$_2$O$_3$ (amorp)	69.6202	Boric oxide	-299.84	-1254.53	[3]
BaO (g)	153.339	Barium oxide	-28.	-117.	[6]
BaO (c)	153.339	Barium oxide	-132.3	-553.5	[6]
BaO$_2$ (c)	169.339	Barium peroxide	-151.6	-634.3	[6]
Ba$_2$O (g)	290.679	Dibarium monoxide	-72.	-301.	[6]
Ba$_2$O (c)	290.679	Dibarium monoxide	-147.1	-615.5	[6]
Ba$_2$O$_2$ (g)	306.679	Dibarium dioxide	-135.	-565.	[6]
BeO (g)	25.0116	Beryllium oxide	28.	117.	[6]
BeO (c)	25.0116	Beryllium oxide	-145.7	-609.6	[6]
Be$_2$O (g)	34.0238	Diberyllium monoxide	-20.	-84.	[6]
(BeO)$_2$ (g)	50.0232	Beryllium oxide, dimer	-103.	-431.	[6]
(BeO)$_3$ (g)	75.0348	Beryllium oxide, trimer	-260.	-1088.	[6]
(BeO)$_4$ (g)	100.0464	Beryllium oxide, tetramer	-391.	-1636.	[6]
(BeO)$_5$ (g)	125.0580	Beryllium oxide, pentamer	-518.	-2167.	[6]
(BeO)$_6$ (g)	150.0696	Beryllium oxide, hexamer	-651.	-2724.	[6]
Bi$_2$O$_3$ (c)	465.9582	Bismuth trioxide, Bismite	-137.16	-573.88	[3]
BrO (g)	95.9084	Bromine monoxide	30.06	125.77	[3]
BrO$_2$ (c)	111.9078	Bromine dioxide	11.6	48.5	[3]

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

formula (state)	formula weight (g mol⁻¹)	name	Enthalpy of formation, ΔHf° kcal mol⁻¹	kJ mol⁻¹	Ref.
CO (g)	28.0106	Carbon monoxide	-26.416	-110.524	[3]
CO_2 (g)	44.0100	Carbon dioxide	-94.051	-393.509	[3]
C_3O_2 (g)	68.0323	Carbon suboxide	-22.38	-93.64	[7]
C_3O_2 (liq)	68.0323	Carbon suboxide	-28.03	-117.28	[7]
CaO (c)	56.079	Calcium oxide	-151.79	-635.09	[6]
CaO_2 (c)	72.079	Calcium peroxide	-156.0	-652.7	[6]
CdO (c)	128.399	Cadmium oxide, Monteponite	-61.7	-258.2	[3]
CeO_2 (c)	172.119	Cerium dioxide, Cerium (IV) oxide, Cerianite, Ceria	-260.2	-1088.7	[12]
Ce_2O_3 (c, hexagonal)	328.238	Cerium trioxide, Cerium (III) oxide	-428.4	-1792.4	[12]
ClO (g)	51.4524	Chlorine monoxide	24.34	101.84	[3]
ClO_2 (g)	67.4518	Chlorine dioxide	24.5	102.5	[3]
ClO_3 (g)	83.4512	Chlorine trioxide	37.	155.	[3]
Cl_2O (g)	86.9054	Dichlorine monoxide	19.2	80.3	[3]
Cl_2O_7 (g)	182.9018	Chlorine heptoxide	65.0	272.0	[3]
Cl_2O_7 (liq)	182.9018	Chlorine heptoxide	56.9	238.1	[3]
CoO (c)	74.9326	Cobaltous oxide, Cobalt (II) oxide	-56.87	-237.94	[4]
Co_3O_4 (c)	240.7972	Cobalt (II,III) oxide	-213.	-891.	[4]
CrO_2 (c)	83.9948	Chromium dioxide	-143.	-598.	[4]
CrO_3 (g)	99.9942	Chromium tioxide, Chromic anhydride "Chromic acid"	-92.2	-385.8	[4]

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

formula (state)	formula weight (g mol^{-1})	name	Enthalpy of formation, $\Delta Hf°$ kcal mol^{-1}	kJ mol^{-1}	Ref.
CrO_3 (c)	99.9942	Chromium trioxide, chromic anhydride "Chromic acid"	-140.9	-589.5	[4]
Cr_2O_3 (c)	151.9902	Chromium sesquioxide, Eskolaite	-272.4	-1139.7	[4]
Cr_3O_4 (c)	219.9856	Chromium (II,III) oxide	-366.	-1531.	[4]
Cs_2O (c)	281.8094	Dicesium oxide	-75.9	-317.6	[2]
Cs_2O_2 (c)	297.8088	Dicesium dioxide	-96.2	-402.5	[2]
Cs_2O_3 (c)	313.8082	Dicesium trioxide	-111.2	-465.3	[2]
Cs_2O_4 (c)	329.8076	Dicesium tetroxide	-124.2	-519.6	[2]
CuO (c)	79.539	Cupric oxide, Copper (II) oxide Tenorite	-37.6	-157.3	[4]
Cu_2O (liq)	143.0794	Cuprous oxide	-32.0	-133.9	[7]
Cu_2O (c)	143.079	Cuprous oxide, Copper (I) oxide Cuprite	-40.3	-168.6	[4]
Dy_2O_3 (c, cubic)	372.998	Dysprosium trioxide, Dysprosium (III) oxide	-446.8	-1869.4	[12]
Er_2O_3 (c, cubic)	382.518	Erbium trioxide, Erbium (III) oxide	-453.6	-1897.9	[12]
Eu_2O_3 (c, cubic)	351.918	Europium trioxide, Europium (III) oxide	-389.6	-1630.1	[12]
Eu_2O_3 (c, mono-clinic)	351.918	Europium trioxide, Europium (III) oxide	-393.9	-1648.1	[12]
FO (g)	34.9978	Fluorine monoxide	41.	171.	[3]
F_2O (g)	53.9962	Oxygen difluoride, Difluorine oxide	-5.2	-21.8	[3]
F_2O_2 (g)	69.9956	Dioxygen difluoride, Fluorine dioxide	4.3	18.0	[3]
F_2O_3 (g)	85.9950	Difluorine trioxide	3.8	15.9	[3]

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

formula (state)	name	formula weight (g mol^{-1})	Enthalpy of formation, ΔH_f° kcal mol^{-1}	kJ mol^{-1}	Ref.
Fe$_{0.947}$O (c)	Ferrous oxide, Wüstite	68.8865	-63.64	-266.27	[4]
FeO (c)	Ferrous oxide, Iron (II) oxide, (Fictive)	71.8464	-65.0	-272.0	[4]
Fe$_2$O$_3$ (c)	Ferric oxide, Iron (III) oxide, Hematite	159.6922	-197.0	-824.2	[4]
Fe$_3$O$_4$ (c)	Iron (II,III) oxide, Magnetite	231.5386	-267.3	-1118.4	[4]
GaO (g)	Gallium monoxide	85.719	66.8	279.5	[3]
Ga$_2$O (g)	Digallium monoxide	155.439	-21.	-88.	[3]
Ga$_2$O (c)	Digallium monoxide	155.439	-85.	-356.	[3]
Ga$_2$O$_3$(c)	Gallium sesquioxide	187.438	-260.3	-1089.1	[3]
Gd$_2$O$_3$ (c, monoclinic)	Gadolinium trioxide, Gadolinium (III) oxide	362.498	-434.9	-1819.6	[12]
GeO (g)	Germanium monoxide	88.589	-11.04	-46.19	[3]
GeO (c, brown)	Germanium monoxide	88.589	-50.7	-212.1	[3]
GeO (c, hexagonal)	Germanium dioxide	104.589	-131.7	-551.0	[3]
GeO$_2$ (amorp)	Germanium dioxide	104.589	-128.4	-537.2	[3]
Ge$_2$O$_2$ (g)	Digermanium dioxide	177.179	-112.	-469.	[3]
Ge$_3$O$_3$ (g)	Trigermanium trioxide	265.768	-212.	-887.	[3]
HO (g)	Hydroxyl	17.0074	9.31	38.95	[3]
HO$_2$ (g)	Hydroperoxyl	33.0068	5.	21.	[3]
H$_2$O (g)	Water	18.0153	-57.796	-241.818	[3]

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

formula (state)	formula weight (g mol^{-1})	name	Enthalpy of formation, $\Delta Hf°$		
			kcal mol^{-1}	kJ mol^{-1}	Ref.
H_2O (liq)	18.0153	Water	-68.315	-285.830	[3]
H_2O (c)	18.0153	Water (ice, metastable)	-66.879	-279.822	[1]
H_2O_2 (g)	37.0147	Hydrogen peroxide	-32.58	-136.31	[3]
H_2O_2 (liq)	34.0147	Hydrogen peroxide	-44.88	-187.78	[3]
HfO (g)	194.489	Hafnium monoxide	12.	50.	[5]
HfO_2 (c)	210.489	Hafnium dioxide, Hafnia	-273.6	-1144.7	[5]
HgO (c, hexagonal)	216.589	Mercuric oxide, Mercury (II) oxide	-21.4	-89.5	[4]
HgO (c, red, orthoorhombic)	216.589	Mercuric oxide, Mercury (II) oxide, Montroydite	-21.71	-90.83	[4]
HgO (c, yellow, orthoorhombic)	216.589	Mercuric oxide, Mercury (II) oxide, Montroydite	-21.62	-90.46	[4]
Ho_2O_3 (c, cubic)	377.8582	Holmium trioxide, Holmium (III) oxide	-449.5	-1880.7	[12]
IO (g)	142.9038	Iodine monoxide	41.84	175.06	[3]
I_2O_5 (c)	333.8058	Iodine pentoxide	-37.78	-158.07	[3]
InO (g)	130.819	Indium monoxide	92.5	387.0	[3]
In_2O_3 (c)	277.638	Indium sesquioxide	-221.27	-925.79	[3]
IrO_2 (c)	224.20	Iridium dioxide	-65.5	-274.0	[4]
IrO_3 (g)	240.20	Iridium trioxide	1.9	7.9	[4]
KO_2 (c)	71.1008	Potassium superoxide	-68.0	-284.5	[8]
K_2O (c)	94.2034	Potassium oxide	-86.8	-363.2	[7]
K_2O_2 (c)	110.2028	Potassium peroxide	-118.5	-495.8	[7]

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

formula (state)	name	formula weight (g mol^{-1})	Enthalpy of formation, $\Delta H_f°$ kcal mol^{-1}	kJ mol^{-1}	Ref.
La$_2$O (g)	Dilanthanum monoxide	293.819	-3.2	-13.4	[12]
La$_2$O$_2$ (g)	Dilanthanum dioxide	309.819	-146.6	-613.4	[12]
La$_2$O$_3$ (c, hexagonal)	Lanthanum trioxide, Lanthanum (III) oxide	325.818	-428.7	-1793.7	[12]
Li$_2$O (g)	Lithium oxide	29.8774	-39.9	-166.9	[7]
Li$_2$O (c)	Lithium oxide	29.8774	-143.1	-598.7	[7]
Li$_2$O$_2$ (c)	Lithium peroxide	45.8768	-151.2	-632.6	[7]
Lu$_2$O$_3$ (c, cubic)	Lutetium trioxide, Lutetium (III) oxide	397.938	-448.9	-1878.2	[12]
MgO (c, macro-crystal)	Magnesium oxide, Periclase	40.3114	-143.81	-601.70	[6]
MgO (c, micro-crystal)	Magnesium oxide	40.3114	-142.92	-597.98	[6]
MnO (g)	Manganese (II) oxide, Manganosite	70.9374	29.6	123.8	[4]
MnO (c)	Manganese (II) oxide, Manganosite	70.9374	-92.07	-385.22	[4]
MnO$_2$ (c)	Manganese dioxide, Pyrolusite	86.9368	-124.29	-520.03	[4]
Mn$_2$O$_3$ (c)	Manganese sesquioxide, Braunite, Bixbyite	157.8742	-229.2	-959.0	[4]
Mn$_3$O$_4$ (c)	Manganese (II,III) oxide, Hausmannite	228.8116	-331.7	-1387.8	[4]
MoO (g)	Molybdenum monoxide	111.939	101.	422.	[4]
MoO$_2$ (g)	Molybdenum dioxide	127.939	3.	13.	[4]
MoO$_2$ (c)	Molybdenum dioxide	127.939	-140.76	-588.94	[4]
MoO$_3$ (g)	Molybdenum trioxide, Molybdic anhydride, Molybdite	143.939	-78.	-326.	[4]

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

formula (state)	formula weight (g mol^{-1})	name	Enthalpy of formation, ΔHf° kcal mol^{-1}	kJ mol^{-1}	Ref.
MoO$_3$ (c)	143.939	Molybdenum trioxide, Molybdic anhydride, Molybdite	-178.08	-745.09	[4]
(MoO$_3$)$_2$ (g)	287.876	Molybdenum trioxide, dimer	-271.	-1134.	[4]
(MoO$_3$)$_3$ (g)	431.815	Molybdenum trioxide, trimer	-451.	-1887.	[4]
(MoO$_3$)$_4$ (g)	575.753	Molybdenum trioxide, tetramer	-618.	-2586.	[4]
(MoO$_3$)$_5$ (g)	719.691	Molybdenum trioxide, pentamer	-783.	-3276.	[4]
NO (g)	30.0061	Nitric oxide	21.57	90.25	[3]
NO$_2$ (g)	46.0055	Nitrogen dioxide, Nitrogen peroxide	7.93	33.18	[3]
N$_2$O (g)	44.0128	Nitrous oxide	19.61	82.05	[3]
N$_2$O$_3$ (g)	76.0116	Dinitrogen trioxide, Nitrous anhydride	20.01	83.72	[3]
N$_2$O$_3$ (liq)	76.0116	Dinitrogen trioxide, Nitrous anhydride	12.02	50.29	[3]
N$_2$O$_4$ (g)	92.0110	Dinitrogen tetroxide	2.19	9.16	[3]
N$_2$O$_4$ (liq)	92.0110	Dinitrogen tetroxide	-4.66	-19.50	[3]
N$_2$O$_5$ (g)	108.0104	Nitrogen pentoxide, Nitric anhydride	2.7	11.3	[3]
N$_2$O$_5$ (c)	108.0104	Nitrogen pentoxide, Nitric anhydride	-10.3	-43.1	[3]
NaO$_2$ (c)	54.9886	Sodium superoxide	-62.3	-260.7	[7]
Na$_2$O (c)	61.9790	Sodium oxide	-99.9	-418.0	[7]
Na$_2$O$_2$ (c)	77.9784	Sodium peroxide	-122.66	-513.21	[7]
NbO (g)	108.9054	Niobium monoxide	51.	213.	[5]
NbO (c)	108.9054	Niobium monoxide	-97.0	-405.8	[5]
NbO$_2$ (g)	124.9048	Niobium dioxide	-51.3	-214.6	[5]
NbO$_2$ (c)	124.9048	Niobium dioxide	-190.3	-796.2	[5]

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula (state) | formula weight (g mol^{-1}) | name | Enthalpy of formation, $\Delta Hf°$ | | Ref. |
			kcal mol^{-1}	kJ mol^{-1}	
Nb$_2$O$_5$ (c)	265.809	Niobium pentoxide	-454.0	-1899.5	[5]
Nd$_2$O$_3$ (c, hexagonal)	336.478	Neodymium trioxide, Neodymium (III) oxide	-432.36	-1808.99	[12]
NiO (c)	74.709	Nickel monoxide, Bunsenite	-57.3	-239.7	[4]
Ni$_2$O$_3$ (c)	165.418	Nickel sesquioxide, Nickel (III) oxide	-117.0	-489.5	[4]
NpO$_2$ (c)	(269.0488)^a	Neptunium dioxide	-256.7	-1074.0	[9]
O (g)	15.9994	Oxygen, monatomic	59.553	249.170	[3]
O$_2$ (g)	31.9988	Oxygen	0	0	[3]
O$_3$ (g)	47.9982	Ozone	34.1	142.7	[3]
OsO$_3$ (g)	238.20	Osmium trioxide	-67.8	-283.7	[4]
OsO$_4$ (g)	254.20	Osmium tetroxide	-80.6	-337.2	[4]
OsO$_4$ (c,white)	254.20	Osmium tetroxide	-92.2	-385.8	[4]
OsO$_4$ (c,yellow)	254.20	Osmium tetroxide	-94.2	-394.1	[4]
P$_4$O$_6$ (g)	219.8916	Phosphorus sesquioxide, Phosphorus trioxide	-512.5	-2144.3	[7]
P$_4$O$_6$ (c)	219.8916	Phosphorus trioxide, Phosphorous anhydride	-392.0	-1640.1	[3]
P$_4$O$_{10}$ (g)	283.8892	Phosphorus pentoxide, Phosphoric anhydride	-677.4	-2834.2	[7]
P$_4$O$_{10}$ (c)	283.8892	Phosphorus pentoxide, Phosphoric anhydride	-713.2	-2984.0	[3]

^{a}Enthalpy of formation and formula weight are based on an atomic weight of 237.05 for Np, as used by the authors of reference [9].

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

formula (state)	name	formula weight ($g\ mol^{-1}$)	Enthalpy of formation, $\Delta Hf°$ $kcal\ mol^{-1}$	Enthalpy of formation, $\Delta Hf°$ $kJ\ mol^{-1}$	Ref.
P_4O_{10} (amorp)	Phosphorus pentoxide, Phosphoric anhydride	283.8892	-727.	-3042.	[3]
PbO (g)	Lead monoxide	223.189	-11.48	-48.03	[7]
PbO (c, red)	Lead monoxide, Litharge	223.189	-52.34	-218.99	[3]
PbO (c, yellow)	Lead monoxide, Massicot	223.189	-51.94	-217.32	[3]
PbO_2 (c)	Lead dioxide, Plattnerite	239.189	-66.3	-277.4	[3]
Pb_3O_4 (c)	Lead oxide, Minium	685.568	-171.7	-718.4	[3]
PdO (g)	Palladium monoxide	122.40	83.4	348.9	[4]
PdO (c)	Palladium monoxide	122.40	-20.4	-85.4	[4]
PtO_2 (g)	Platinum dioxide	227.089	41.0	171.5	[4]
Pt_3O_4 (c)	Platinum (II,III) oxide	649.268	-39.	-163.	[4]
PuO_2 (c)	Plutonium dioxide	$(271.0998)^b$	-252.87	-1058.01	[10]
RaO (c)	Radium oxide	242.019	-125.	-523.	[6]
Rb_2O (c)	Rubidium oxide	186.939	-78.9	-330.1	[2]
Rb_2O_2 (c)	Dirubidium dioxide	202.939	-101.7	-425.5	[2]
Rb_2O_3 (c)	Dirubidium trioxide	218.938	-116.7	-488.3	[2]
Rb_2O_4 (c)	Dirubidium tetroxide	234.938	-126.2	-528.0	[2]
ReO_3 (c)	Rhenium trioxide	234.20	-144.6	-605.0	[4]
Re_2O_7 (g)	Rhenium heptoxide	484.40	-263.	-1100.	[4]
Re_2O_7 (c)	Rhenium heptoxide	484.40	-296.4	-1240.1	[4]
RhO (g)	Rhodium monoxide	118.9044	92.	385.	[4]
RhO_2 (g)	Rhodium dioxide	134.9038	44.	184.	[4]

^{b}Enthalpy of formation and formula weight are based on an atomic weight of 239.1 for Pu, as used by the authors of reference [10].

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

formula (state)	formula weight (g mol⁻¹)	name	Enthalpy of formation, $\Delta H_f°$		Ref.
			kcal mol⁻¹	kJ mol⁻¹	
Rh_2O_3 (c)	253.8082	Rhodium sesquioxide	-82.	-343.	[4]
RuO_2 (c)	133.069	Ruthenium dioxide	-72.9	-305.0	[4]
RuO_3 (g)	149.068	Ruthenium trioxide	-18.7	-78.2	[4]
RuO_4 (g)	165.068	Ruthenium tetroxide	-44.0	-184.1	[4]
RuO_4 (liq)	165.068	Ruthenium tetroxide	-54.6	-228.4	[4]
RuO_4 (c)	165.068	Ruthenium tetroxide	-57.2	-239.3	[4]
SO (g)	48.0634	Sulfur monoxide	1.496	6.259	[3]
SO_2 (g)	64.0628	Sulfur dioxide	-70.944	-296.830	[3]
SO_2 (liq)	64.0628	Sulfur dioxide	-76.6	-320.5	[3]
SO_3 (g)	80.0622	Sulfur trioxide	-94.58	-395.72	[3]
SO_3 (liq)	80.0622	Sulfur trioxide	-105.41	-441.04	[3]
SO_3 (c)	80.0622	Sulfur trioxide	-108.63	-454.51	[3]
SbO (g)	137.749	Antimony monoxide	47.67	199.45	[3]
Sb_2O_4 (c)	307.498	Antimony tetroxide, Cerrantite	-216.9	-907.5	[3]
Sb_2O_5 (c)	323.497	Antimony pentoxide	-232.3	-971.9	[3]
Sb_4O_6 (c, cubic)	582.996	Antimony trioxide, Senarmontite	-344.3	-1440.6	[3]
Sb_4O_6 (c, orthorhombic)	582.996	Antimony trioxide, Valentinite	-338.7	-1417.1	[3]
Sb_6O_{13} (c)	938.492	Antimony (III,IV) oxide	-670.6	-2805.8	[3]
ScO (g)	60.955	Scandium monoxide	-13.68	-57.24	[5]
Sc_2O (g)	105.911	Discandium monoxide	-6.9	-28.9	[5]

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

formula (state)	name	formula weight ($g\ mol^{-1}$)	Enthalpy of formation, $\Delta Hf°$ $kcal\ mol^{-1}$	$kJ\ mol^{-1}$	Ref.
Sc_2O_3 (c)	Scandium trioxide, Scandia, Scandium sesquioxide	137.910	-456.22	-1908.82	[5]
SeO (g)	Selenium monoxide	94.959	12.75	53.35	[3]
SeO_2 (c)	Selenium dioxide	110.959	-53.86	-225.35	[3]
SeO_3 (c)	Selenium trioxide	126.958	-39.9	-166.9	[3]
Se_2O_5 (c)	Diselenium pentoxide	237.917	-97.6	-408.4	[3]
SiO (g)	Silicon monoxide	44.0854	-23.8	-99.6	[3]
SiO_2 (g)	Silicon dioxide	60.0848	-77.	-322.	[3]
SiO_2 (c, crysto-balite)	Silicon dioxide, Crystobalite	60.0848	-217.37	-909.48	[3]
SiO_2 (c, quartz)	Silicon dioxide, Quartz	60.0848	-217.72	-910.94	[3]
SiO_2 (c, tri-dymite)	Silicon dioxide, Tridymite	60.0848	-217.27	-909.06	[3]
SiO_2 (c)	Silicon dioxide, Coesite	60.0848	-216.44	-905.58	[1]
SiO_2 (c)	Silicon dioxide, Stishovite	60.0848	-205.86	-861.32	[1]
SiO_2 (amorp)	Silicon dioxide, Silica glass	60.0848	-215.94	-903.49	[3]
Sm_2O_3 (c, mono-clinic)	Samarium trioxide, Samarium (III) oxide	348.698	-433.7	-1814.6	[12]
SnO (c)	Tin monoxide	134.689	-68.3	-285.8	[3]
SnO_2 (c)	Tin dioxide, Cussiterite	150.689	-138.8	-580.7	[3]
SrO (g)	Strontium monoxide	103.619	-2.	-8.	[6]
SrO (c)	Strontium monoxide	103.619	-141.5	-592.0	[6]

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

formula (state)	formula weight (g mol^{-1})	name	Enthalpy of formation, $\Delta Hf°$ kcal mol^{-1}	kJ mol^{-1}	Ref.
SrO$_2$ (c)	119.619	Strontium peroxide	-151.4	-633.5	[6]
Sr$_2$O (g)	191.239	Distrontium monoxide	-56.	-234.	[6]
Sr$_2$O (c)	191.239	Distrontium monoxide	-154.7	-647.3	[6]
TaO (g)	196.9474	Tantalum monoxide	60.	251.	[5]
TaO$_2$ (g)	212.9468	Tantalum tetroxide	-41.	-172.	[5]
Ta$_2$O$_5$ (c,β)	441.8930	Tantalum pentoxide	-489.0	-2046.0	[5]
TbO$_2$ (c)	190.9228	Terbium dioxide, Terbium (IV) oxide	-232.2	-971.5	[12]
Tb$_2$O$_3$ (c, cubic)	365.8462	Terbium trioxide, Terbium (III) oxide	-445.2	-1862.7	[12]
Tc$_2$O$_7$ (c)	309.8078	Technetium heptoxide	-266.	-1113.	[4]
TeO (g)	143.599	Tellurium monoxide	15.6	65.3	[3]
TeO$_2$ (c)	159.599	Tellurium dioxide, Tellurite	-77.1	-322.6	[3]
ThO$_2$ (c)	264.0368	Thorium dioxide, Thorianite, Thoria	-293.20	-1226.75	[1]
TiO (g)	63.899	Titanium monoxide	4.	17.	[5]
TiO (c,α)	63.899	Titanium monoxide	-124.2	-519.6	[5]
TiO$_2$ (g)	79.899	Titanium dioxide	-60.	-251.	[5]
TiO$_2$ (c)	79.899	Titanium dioxide, Anatase Octahedrite	-224.6	-939.7	[5]
TiO$_2$ (c)	79.899	Titanium dioxide, Brookite	-225.1	-941.8	[5]
TiO$_2$ (c)	79.899	Titanium dioxide, Rutile	-225.8	-944.7	[5]
TiO$_2$ (amorp)	79.899	Titanium dioxide	-210.	-879.	[5]

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

formula (state)	name	formula weight ($g\ mol^{-1}$)	Enthalpy of formation, ΔHf°		Ref.
			$kcal\ mol^{-1}$	$kJ\ mol^{-1}$	
Ti_2O_3 (c)	Titanium sesquioxide	143.798	-363.5	-1520.9	[5]
Ti_3O_5 (c)	Tritanium pentoxide	223.697	-587.8	-2459.4	[5]
Tl_2O (c)	Thallous oxide, Thallium (I) oxide	424.7394	-42.7	-178.7	[3]
Tm_2O_3 (c, cubic)	Thulium trioxide, Thulium (III) oxide	385.8662	-451.4	-1888.7	[12]
UO_2 (c)	Uranium dioxide, Uraninite	270.029	-259.20	-1084.49	[1]
UO_3 (c,α)	Uranium trioxide	286.0282	-291.3	-1218.8	[11]
UO_3 (c,β)	Uranium trioxide	286.0282	-292.0	-1221.7	[11]
UO_3 (c,γ)	Uranium trioxide	286.0282	-292.0	-1225.9	[11]
U_3O_7 (c,β)	Triuranium heptoxide	826.0858	-819.1	-3427.1	[11]
U_3O_8 (c)	Triuranium octoxide, Pitchblende	842.0852	-854.4	-3574.8	[11]
U_4O_9 (c)	Tetrauranium nonoxide	1094.1146	-1078.0	-4510.4	[11]
VO (g)	Vanadium monoxide	66.9414	25.	105.	[5]
VO (c)	Vanadium monoxide	66.9414	-103.2	-431.8	[5]
VO_2 (g)	Vanadium dioxide	82.9408	-57.	-238.	[5]
V_2O_3 (c)	Vanadium sesquioxide, Vanadium tri-oxide, Karelianite	149.8822	-293.5	-1228.0	[5]
V_2O_4 (c,α)	Vanadium tetroxide	165.8816	-341.1	-1427.2	[5]
V_2O_5 (c)	Vanadium pentoxide	181.8810	-370.6	-1550.6	[5]
V_3O_5 (c)	Trivanadium pentoxide	232.8230	-465.	-1946.	[5]
V_4O_7 (c)	Tetravanadium heptoxide	315.7638	-635.	-2657.	[5]
V_6O_{13} (c)	Hexavanadium tridecaoxide	513.6442	-1062.	-4443.	[5]

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

formula (state)	name	formula weight ($g\ mol^{-1}$)	Enthalpy of formation, $\Delta Hf°$		
			$kcal\ mol^{-1}$	$kJ\ mol^{-1}$	Ref.
WO (g)	Tungsten monoxide	199.849	108.	452.	[4]
WO$_2$ (g)	Tungsten dioxide	215.849	11.	46.	[4]
WO$_2$ (c)	Tungsten dioxide	215.849	-140.94	-589.69	[4]
WO$_3$ (g)	Tungsten trioxide	231.848	-71.	-297.	[4]
WO$_3$ (c)	Tungsten trioxide, Wolframite	231.848	-201.45	-842.87	[4]
(WO$_3$)$_2$ (g)	Tungsten trioxide, dimer	463.696	-277.	-1159.	[4]
(WO$_3$)$_3$ (g)	Tungsten trioxide, trimer	695.545	-468.	-1958.	[4]
(WO$_3$)$_4$ (g)	Tungsten trioxide, tetramer	927.393	-649.	-2715.	[4]
Yb$_2$O$_3$ (c, cubic)	Ytterbium trioxide, Ytterbium (III) oxide	394.078	-433.7	-1814.6	[12]
YO (g)	Yttrium monoxide	104.9044	-9.3	-38.9	[5]
Y$_2$O (g)	Diyttrium monoxide	193.8094	1.0	4.2	[5]
Y$_2$O$_2$ (g)	Diyttrium dioxide	209.8088	-127.4	-533.0	[5]
Y$_2$O$_3$ (c)	Yttrium trioxide, Yttria	225.8082	-455.38	-1095.31	[5]
ZnO (c)	Zinc oxide, Zincite	81.369	-83.24	-348.28	[3]
ZrO (g)	Zirconium monoxide, Zirconium (II) oxide	107.219	15.	63.	[5]
ZrO$_2$ (g)	Zirconium dioxide, Zirconium (IV) oxide	123.219	-75.	-314.	[5]
ZrO$_2$ (c, α monoclinic)	Zirconium dioxide, Zirconium (IV) oxide, Baddeleyite	123.219	-263.04	-1100.56	[5]

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References to Table III

[1] Robie, R. A., and Waldbaum, D. R., "Thermodynamic Properties of Minerals and Related Substances at 298.15 K (25.0°C) and One Atmosphere (1.013 Bars) Pressure and at Higher Temperatures," U. S. Department of Interior, Geological Survey Bulletin 1259, (1968).

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[7] Stull, D. R., and Prophet, H., et al., JANAF Thermochemical Tables, 2nd Edition, NSRDS-NBS-37, 1141 pp. (June 1971), (U. S. Government Printing Office, Washington, D. C. 20402).

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26.0 Appendix

26.1 Symbols for Thermodynamic Quantities, (IUPAC). (1) (2)

T	thermodynamic temperature (absolute temperature)
t, θ	Celsius temperature
R	molar gas constant
k	Boltzmann constant
q, Q	heat
w, W	work
U, (E)	internal energy
H	enthalpy: $H = U + pV$
S	entropy
A	Helmholtz energy: $A = U - TS$
J	Massieu function: $J = -A/T$
G	Gibbs energy: $G = H - TS$, (3) (see footnote (3), page 202)
Y	Planck function: $Y = -G/T$
Z	compressibility factor: $Z = pV/nRT$
C	heat capacity
c	specific heat capacity (heat capacity divided by mass)
γ, (k)	heat capacity ratio: C_p/C_v
μ	Joule-Thomson coefficient
λ, k	thermal conductivity
a	thermal diffusivity: $a = \lambda/\rho C_p$

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(1) Symbols adopted by the International Union of Pure and Applied Chemistry (IUPAC), 1969.

(2) Symbols in parentheses are alternates, accepted but not recommended by IUPAC. See Section 25.2 for other commonly used symbols and names of quantities not accepted by IUPAC.

h	coefficient of heat transfer
α	cubic expansion coefficient: $\alpha = (\partial V/\partial T)_p/V$
k	isothermal compressibility: $k = -(\partial V/\partial p)_T/V$
β	pressure coefficient: $\beta = (\partial p/\partial T)_V$
μ_B	chemical potential of substance B
λ_B	absolute activity of substance B: $\lambda_B = \exp(\mu_B/RT)$
f, (p*)	fugacity
Π	osmotic pressure
I	ionic strength: $I = \frac{1}{2} \Sigma_i m_i z_i^2$ or $I = \frac{1}{2} \Sigma_i c_i z_i^2$
a_B	activity, relative activity of substance B
f_B	activity coefficient, mole fraction basis
γ_B	activity coefficient, molality basis
y_B	activity coefficient, concentration basis
$\emptyset$	osmotic coefficient

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(3) The Gibbs energy is frequently called free energy, Gibbs free
energy, or Gibbs function. The commonly encountered term
free energy in American work on thermodynamics almost invariably
refers to Gibbs energy. This usage of the term free energy and
the symbol F are being discouraged by the IUPAC because of confusion
with the Helmholtz energy and the common European usage of F for
the latter.

26.2 Selected Symbols for Other Quantities needed in Thermodynamics
(IUPAC)[1] (see footnote (1), page 201)

A, S	area
V	volume
t	time
m	mass

ρ density (mass divided by volume)

P pressure

A_r relative atomic mass (also called "atomic weight")

M_r relative molecular mass (also called "molecular weight")

L, N_A Avogadro constant

N number of molecules

n, (ν) amount of substance

x_B, y_B mole fraction of substance B: $x_B = n_B / \Sigma_i n_i$

w_B mass fraction of substance B

ϕ_B volume fraction of substance B

m_B molality of solute substance B (amount of B divided by the mass of solvent)

c_B, $[B]$ concentration of substance B (amount of B divided by the volume of the solution)

ρ_B mass concentration of substance B (mass of B divided by the volume of the solution)

ν_B stoichiometric coefficient of substance B (negative for reactants, positive for products).

(The general equation for a chemical reaction is -- $\Sigma_B \nu_B B = 0$, [Example: for the reaction $H_2O \rightarrow H_2 + \frac{1}{2}O_2$, $H_2 + \frac{1}{2}O_2 - H_2O = 0$]

ζ extent of reaction: $(d\zeta = dn_b / \nu_B)$

K equilibrium constant

α degree of dissociation

z_B charge number of an ion B (positive for cations, negative for anions)

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26.3   Units of Measurement - International System (SI)

SI - Base Units and Supplementary Units

quantity	name of unit	symbol
length	metre	m
mass	kilogram	kg
time	second	s
temperature	kelvin	K
electric current	ampere	A
luminous intensity	candela	cd
amount of substance	mole	mol
plane angle	radian	rad
solid angle	steradian	sr

26.4   Definitions of the SI Base Units

metre: The metre is the length equal to 1 650 763.73 wavelengths in vacuum of the radiation corresponding to the transition between the levels $2p_{10}$ and $5d_5$ of the krypton -86 atom.

kilogram: The kilogram is equal to the mass of the international prototype of the kilogram.

second: The second is the duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the cesium-133 at

kelvin: The kelvin is the fraction 1/273.16 of the thermodynamic

temperature of the triple point of water. The kelvin is used

both for thermodynamic temperature and for thermodynamic

temperature interval.

ampere: The ampere is that constant current which, if maintained in

two straight parallel conductors of infinite length, of

negligible cross-section, and placed 1 metre apart in vacuum,

would produce between these conductors a force equal to 2×10^{-7}

newton per metre of length.

candela: The candela is the luminous intensity, in the perpendicular

direction, of a surface of 1/600 000 square metre of a black

body at the temperature of freezing platinum under a pressure

of 101 325 newtons per square metre.

mole: The mole is the amount of substance of a system which contains

as many elementary entities as there are carbon atoms in

0.012 kilogram of carbon-12.

Note: The elementary entities must be specified and may be atoms,

molecules, ions, electrons, other particles, or specified groups

of such particles.

26.5 Prefixes

SI Symbol	Prefix name	Multiplication factor
T	tera	10^{12}
G	giga	10^{9}
M	mega	10^{6}
k	kilo	10^{3}
h	hecto	10^{+2}
da	deka	10^{+1}
d	deci	10^{-1}
c	centi	10^{-2}
m	milli	10^{-3}
μ	micro	10^{-6}
n	nano	10^{-9}
p	pico	10^{-12}
f	femto	10^{-15}
a	atto	10^{-18}

26.6 <u>SI Derived Units</u> (partial listing)

	Symbol for SI unit	Definition of SI unit	Other Definitions
force	newton	N	$m \cdot kg \cdot s^{-2}$	
pressure	pascal	Pa	$m^{-1} \cdot kg \cdot s^{-2}$	$N \cdot m^{-2}$
energy	joule	J	$m^2 \cdot kg \cdot s^{-2}$	$N \cdot m$
power	watt	W	$m^2 \cdot kg \cdot s^{-3}$	$J \cdot s^{-1}$
electric charge	coulomb	C	$A \cdot s$	
electric potential difference	volt	V	$m^2 \cdot kg \cdot s^{-3} \cdot A^{-1}$	$W \cdot A^{-1}$
electric resistance	ohm	Ω	$m^2 \cdot kg \cdot s^{-3} \cdot A^{-2}$	$V \cdot A^{-1}$
electric conductance	siemens	S	$m^{-2} \cdot kg^{-1} \cdot s^3 \cdot A^2$	$A \cdot V^{-1}$
electric capacitance	farad	F	$m^{-2} \cdot kg^{-1} \cdot s^4 \cdot A^2$	$C \cdot V^{-1}$
magnetic flux	weber	Wb	$m^2 \cdot kg \cdot s^{-2} \cdot A^{-1}$	$V \cdot s$
inductance	henry	H	$m^2 \cdot kg \cdot s^{-2} \cdot A^{-2}$	$Wb \cdot A^{-1}$
magnetic flux density	tesla	T	$kg \cdot s^{-2} \cdot A^{-1}$	$Wb \cdot m^{-2}$
luminous flux	lumen	lm	$cd \cdot sr$	
illumination	lux	lx	$m^{-2} \cdot cd \cdot sr$	
frequency	hertz	Hz	s^{-1}	

26.7 Other Units Exactly Defined in Terms of SI Units (partial listing)

Quantity	Name	Symbol	Definition
length	inch	in.	2.54×10^{-2} m
mass	pound (av.)	lb	0.453 592 37 kg
force	kilogram force	kgf	9.806 65 N
pressure	atmosphere	atm	101 325 $N \cdot m^{-2}$
pressure	torr	Torr	$(101\ 325/760)\ N \cdot m^{-2}$
pressure	millimetre of mercury	mmHg	$13.5951 \times 980.665 \times 10^{-2} N \cdot m^{-2}$
energy	kilowatt-hour	kWh	3.6×10^{6} J
energy	thermochemical calorie***	cal_{th}	4.184 J
energy	IT calorie**	cal_{IT}	4.1868 J
energy	IT British thermal unit**	Btu_{IT}	1055.06 J*
temperature (thermodynamic)	degree Rankine	°R	5/9 K****
temperature	degree Celsius	°C	K*****
temperature	degree Fahrenheit	°F	5/9 K******
volume	litre	l	$10^{-3}\ m^{3}$

* The exact relationship is: 1 Btu_{IT} = (4.1868/1.8)×435.592 37 J.

** IT refers to International Tables (International Steam Tables)

*** The thermochemical calorie is used in tables in this monograph.

**** [T(°R) = 1.8T(K)]; [T(°R) = t(°F) + 459.67]; [T(°R) = 1.8t(°C) + 491.67]

***** [t(°C) = T(K)-273.15]

****** [t(°F) = 1.8t(°C) + 32]

26.8 Physical Constants

Constant	Symbol	Value	Error Limit	Units (SI)	
Speed of light in vacuum	c	2.997 925	3	$\times 10^8$	$m \cdot s^{-1}$
Elementary charge	e	1.602 10	7	10^{19}	C
Avogadro constant	N_A	6.022 52	28	10^{23}	mol^{-1}
Electron rest mass	m_e	9.109 1	4	10^{-31}	kg
Proton rest mass	m_p	1.672 52	8	10^{-27}	kg
Neutron rest mass	m_n	1.674 82	8	10^{-27}	kg
Faraday constant	F	9.648 70	16	10^4	mol^{-1}
Planck constant	h	6.625 6	5	10^{-34}	$J \cdot s$
Rydberg constant	R_∞	1.097 373 1	3	10^{-11}	m^{-1}
Bohr radius	a_o	5.291 67	7	10^{-11}	m
Electron radius	r_e	2.817 77	11	10^{-15}	m
Gas constant	R	8.314 3	12	10^0	$J \cdot K^{-1} \cdot mol^{-1}$
Normal volume perfect gas	V_o	2.241 36	30	10^{-2}	$m^3 \cdot mol^{-1}$
Boltzmann constant	k	1.380 54	18	10^{-23}	$J \cdot K^{-1}$
First radiation constant	c_1	3.741 5	3	10^{-16}	$W \cdot m^2$
Second radiation constant	c_2	1.438 79	19	10^{-2}	$m \cdot K$
Wien displacement constant	b	2.897 8	4	10^{-3}	$m \cdot K$
Stefan-Boltzmann constant	σ	5.669 7	29	10^{-8}	$W \cdot m^{-2} \cdot K^{-4}$
Energy associated with -					
Electron volt	eV	1.602 10	7	$\times 10^{-19}$	$J \cdot (eV)^{-1}$
Frequency (electromagnetic)	e/h	2.418 04	7	10^{14}	$Hz \cdot (eV)^{-1}$
Wavelength (electromagnetic)	ch/e	1.239 81	4	10^{-6}	$eV \cdot m$
Wave number	e/ch	8.065 73	23	10^5	$m^{-1} \cdot (eV)^{-1}$
Kelvin	e/k	1.160 49	16	10^4	$K \cdot (eV)^{-1}$

These physical constants are excerpted from a list
recommended by the National Academy of Sciences and
adopted by the National Bureau of Standards. The
complete list is found in National Bureau of
Standards Technical News Bulletin, October, 1963.

$\pm$ Error limits are approximately 3 standard deviations
and apply to last digits of the value.

26.9   Atomic Weights (Relative Atomic Masses) of the Elements

Name	Symbol	Atomic number	Atomic weight
Actinium	Ac	89	. . . .
Aluminum	Al	13	26.9815
Americium	Am	95	. . . .
Antimony	Sb	51	121.75
Argon	Ar	18	39.948
Arsenic	As	33	74.9216
Astatine	At	85	. . . .
Barium	Ba	56	137.34
Berkelium	Bk	97	. . . .
Beryllium	Be	4	9.0122
Bismuth	Bi	83	208.980
Boron	B	5	10.811[a]
Bromine	Br	35	79.909[b]
Cadmium	Cd	48	112.40
Calcium	Ca	20	40.08
Californium	Cf	98	. . . .
Carbon	C	6	12.01115[a]
Cerium	Ce	58	140.12
Cesium	Cs	55	132.905
Chlorine	Cl	17	35.453[b]
Chromium	Cr	24	51.996[b]
Cobalt	Co	27	58.9332
Copper	Cu	29	63.54
Curium	Cm	96	. . . .
Dysprosium	Dy	66	162.50
Einsteinium	Es	99	. . . .
Erbium	Er	68	167.26
Europium	Eu	63	151.96
Fermium	Fm	100	. . . .
Fluorine	F	9	18.9984
Francium	Fr	87	. . . .
Gadolinium	Gd	64	157.25

Name	Symbol	Atomic number	Atomic weight
Gallium	Ga	31	69.72
Germanium	Ge	32	72.59
Gold	Au	79	196.967
Hafnium	Hf	72	178.49
Helium	He	2	4.0026
Holmium	Ho	67	164.930
Hydrogen	H	1	1.00797[a]
Indium	In	49	114.82
Iodine	I	53	126.9044
Iridium	Ir	77	192.2
Iron	Fe	26	55.847[b]
Krypton	Kr	36	83.80
Lanthanum	La	57	138.91
Lead	Pb	82	207.19
Lithium	Li	3	6.939
Lutetium	Lu	71	174.97
Magnesium	Mg	12	24.312
Manganese	Mn	25	54.9380
Mendelevium	Md	101	....
Mercury	Hg	80	200.59
Molybdenum	Mo	42	95.94
Neodymium	Nd	60	144.24
Neon	Ne	10	20.183
Neptunium	Np	93	....
Nickel	Ni	28	58.71
Niobium	Nb	41	92.906
Nitrogen	N	7	14.0067
Nobelium	No	102	....
Osmium	Os	76	109.2
Oxygen	O	8	15.9994[a]
Palladium	Pd	46	106.4
Phosphorus	P	15	30.9738
Platinum	Pt	78	195.09
Plutonium	Pu	94	....

Name	Symbol	Atomic number	Atomic weight
Polonium	Po	84	....
Potassium	K	19	39.102
Praseodymium	Pr	59	140.907
Promethium	Pm	61	....
Protactinium	Pa	91	....
Radium	Ra	88	....
Radon	Rn	86	....
Rhenium	Re	75	186.2
Rhodium	Rh	45	102.905
Rubidium	Rb	37	85.47
Ruthenium	Ru	44	101.07
Samarium	Sm	62	150.35
Scandium	Sc	21	44.956
Selenium	Se	34	78.96
Silicon	Si	14	28.086[a]
Silver	Ag	47	107.870[b]
Sodium	Na	11	22.9898
Strontium	Sr	38	87.62
Sulfur	S	16	32.064[a]
Tantalum	Ta	73	180.948
Technetium	Tc	43	....
Tellurium	Te	52	127.60
Terbium	Tb	65	158.924
Thallium	Tl	81	204.37
Thorium	Th	90	232.038
Thulium	Tm	69	168.934
Tin	Sn	50	118.69
Titanium	Ti	22	47.90
Tungsten	W	74	183.85
Uranium	U	92	238.03
Vanadium	V	23	50.942
Xenon	Xe	54	131.30
Ytterbium	Yb	70	173.04

Name	Symbol	Atomic number	Atomic weight
Zinc	Zn	30	65.37
Zirconium	Zr	40	91.22

A. E. Cameron and E. Wichers, J. Am. Chem. Soc. 84, 4175-4197 (1962). The element symbols, names, and atomic weights (relative atomic masses) are those recommended by the International Union of Pure and Applied Chemistry (1961). The atomic mass unit is 1/12 the mass of the carbon isotope carbon-12.